Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supporting Information (ESI)

Oxidation of N-trifluormethylthio sulfoximines using $NaOCl \cdot 5H_2O$

Žan Testen and Marjan Jereb*

University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, 1000 Ljubljana, Slovenia

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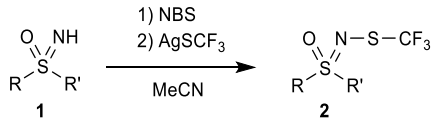
General Information

Chemicals and solvents were obtained from commercial sources. TLC was performed on Merck-60-F254 plates using mixtures of petroleum ether (PE), hexane and ethyl acetate (EtOAc). For flash chromatography, silica gel (63−200µm, 70−230 mesh ASTM; Fluka) was used. Products were characterized by ^{1}H, ^{13}C, and ^{19}F NMR spectroscopy, IR spectroscopy, HRMS, and melting points of solids. All NMR spectra were recorded in $CDCl_3$ using Me_4Si as an internal standard. Chemical shifts are reported in δ (ppm) values relative to δ= 7.26 ppm ($CDCl_3$) for ^{1}H NMR, and to the central line of $CDCl_3$ (δ= 77.16 ppm) for ^{13}C NMR. ^{19}F spectra were referenced to $CFCl_3$ as an external standard at δ= 0.00 ppm. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded with a Bruker Avance III 500 instrument at 500, 126, and 471 MHz, respectively. IR spectra were recorded with a Bruker FTIR Alpha Platinum spectrophotometer. LC-HRMS analyses were performed on a Shimadzu LCMS-IT-TOF system (Kyoto, Japan), composed of a liquid chromatograph Nexera XR hyphenated to a mass spectrometer with an ion trap and time-of-flight tube equipped with an electrospray ionization (ESI) source. The melting points were determined with an OptiMelt MPA100.

Analytical data are given only for the *N*-trifluoromethylthio sulfoximines **2**, which have not yet been reported in the literature.

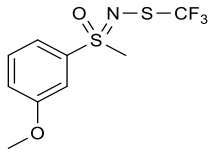
Preparation of *N*-trifluoromethylthio sulfoximines 2

General procedure:

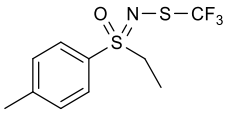


Sulfoximine **1** and dry MeCN (0.1 M) were added to a dried flask. The Flask was equipped with a septum and an argon balloon. *N*-bromosuccinimide (NBS) (1.0 equiv.) was added in one portion with stirring. In a separate dried flask equipped with a septum and argon balloon, a solution of AgSCF3 (0.1 M) was prepared with dry MeCN, which was then slowly transferred with a syringe to the *N*-bromo sulfoximine formed in situ. After complete consumption of the reactant (as judged by TLC), the solvent was removed under reduced pressure and the residue was purified by flash chromatography (EtOAc/hexane).

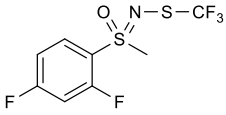
Characterization of obtained *N*-trifuoromethylthio sulfoximines 2



N-trifluoromethylthio-*S*-(3-methoxyphenyl)-*S*-methyl sulfoximine (**2d**). Colorless oil (92%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.53 – 7.48 (m, 1H), 7.48 – 7.43 (m, 1H), 7.42 – 7.38 (m, 1H), 7.23 – 7.18 (m, 1H), 3.88 (s, 3H), 3.27 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.19. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 160.54, 139.16, 130.89, 130.54 (C-F, $^{1}J_{C\text{-}F}$ = 312.7 Hz), 120.80, 120.37, 112.97, 55.93, 43.84. **IR (neat)**: ν 3013, 2932, 2840, 1596, 1579, 1483, 1432, 1407, 1321, 1288, 1222, 1107, 1034, 997, 978, 957, 852, 788, 764, 710, 680 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_9H_{11}F_3NO_2S_2$ 286.0178; Found 286.0177.

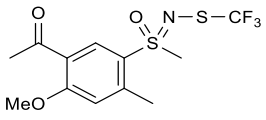


N-trifluoromethylthio-*S*-(*p*-tolyl)-*S*-ethyl sulfoximine (**2e**). Colorless oil (67 %). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.73 – 7.67 (m, 2H), 7.41 – 7.35 (m, 2H), 3.49 – 3.23 (m, 1H), 2.45 (s, 3H), 1.25 (t, *J* = 7.4 Hz, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.30 – (−51.37) (m). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 145.48, 132.54, 130.52 (C-F, $^{1}J_{C\text{-}F}$ = 312.9 Hz), 130.39, 129.10, 50.52, 21.66, 7.46. **IR (neat)**: ν 2982, 2941, 1594, 1492, 1452, 1406, 1239, 1208, 1087, 1041, 960, 814, 775, 729, 692, 617 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{10}H_{13}F_3NOS_2$ 284.0385; Found 284.0388.

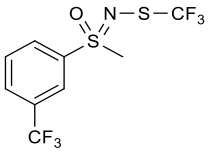


N-trifluoromethylthio-*S*-(2, 4-difluorophenyl)-*S*-methyl sulfoximine (**2i**). Colorless oil (67%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.11 – 7.94 (m, 1H), 7.19 – 7.09 (m, 1H), 7.08 – 6.96 (m, 1H), 3.44 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.14, −97.02 – (−98.78) (m), −101.61 – (−104.79) (m). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 168.28 (d, *J* = 11.5 Hz), 166.21 (d, *J* = 11.5 Hz),

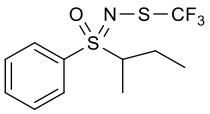
160.64 (d, *J* = 13.1 Hz), 158.59 (d, *J* = 12.9 Hz), 133.71 (d, *J* = 10.9 Hz), 130.31 (C-F, $^{1}J_{C\text{-}F}$ = 312.6 Hz), 121.29 (dd, *J* = 14.7, 3.9 Hz), 112.81 (dd, *J* = 21.9, 3.6 Hz), 106.33, 106.12, 105.92, 43.18 (d, J = 3.9 Hz). **IR (neat)**: ν 3106, 3049, 3020, 2926, 2852, 1601, 1476, 1430, 1406, 1308, 1278, 1236, 1106, 1069, 988, 970, 855, 821, 774, 753, 709, 620 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_8H_7F_3NOS_2$ 291.9884; Found 291.9886.



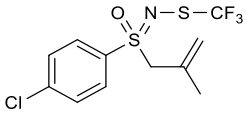
N-trifluoromethylthio-*S*-(5-acetyl-4-methoxy-2-methylphenyl)-*S*-methyl sulfoximine (**2j**). White solid (88%). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 8.37 (s, 1H), 6.93 (s, 1H), 4.00 (s, 3H), 3.30 (s, 3H), 2.69 (s, 3H), 2.60 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −50.67. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 197.18, 162.34 (d, *J* = 1.8 Hz), 144.56, 133.80, 130.57 (C-F, $^{1}J_{C\text{-}F}$ = 312.9 Hz), 128.02 – 127.83 (m), 126.90 – 126.25 (m), 116.20, 56.38, 42.68, 31.75, 21.20. **IR (neat)**: ν 3020, 2933, 1773, 1695, 1672, 1594, 1548, 1480, 1468, 1437, 1402, 1388, 1324, 1271, 1260, 1215, 1172, 1103, 1079, 1038, 1019, 947, 925, 854, 778, 751, 721, 695, 641 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{15}F_3NO_3S_2$ 342.0440; Found 342.0441. Mp = 90.2 – 93.3 °C.



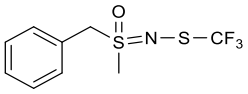
N-trifluoromethylthio-*S*-(3-trifluoromethylphenyl)-*S*-methyl sulfoximine(**2l**). Colorless oil (83%). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 8.21 – 8.17 (m, 1H), 8.13 – 8.07 (m, 1H), 8.02 – 7.93 (m, 1H), 7.83 – 7.74 (m, 1H), 3.33 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −51.00, −63.37. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 139.39, 132.65 (q, *J* = 33.9 Hz), 131.69, 131.09 (q, *J* = 3.4 Hz), 130.35 (C-F, $^{1}J_{C\text{-}F}$ = 312.5 Hz), 130.69, 125.65 (q, *J* = 3.8 Hz), 123.06 (C-F, $^{1}J_{C\text{-}F}$ = 273.0 Hz), 43.73. **IR (neat)**: ν 3080, 3025, 2934, 1748, 1720, 1609, 1433, 1324, 1228, 1097, 1070, 1005, 983, 911, 805, 767, 720, 691, 648 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_8F_6NOS_2$ 323.9946; Found 323.9946.



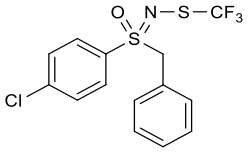
N-(trifluoromethylthio)-*S*-phenyl-*S*-(*sec*-butyl) sulfoximine (**2n**). White solid (71 %). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 7.84 – 7.77 (m, 2H), 7.72 – 7.65 (m, 1H), 7.64 – 7.65 (m, 2H), 3.34 – 3.21 (m, 1H), 2.34 – 1.85 (m, 1H), 1.55 – 1.33 (m, 1H), 1.45 – 1.17 (m, 3H), 1.06 – 0.90 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −51.30 – (−51.37) (m). **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 135.24, 135.07, 133.98 (m), 130.45 (C-F, $^{1}J_{C\text{-}F}$ = 313.3 Hz), 129.80, 129.72, 129.48, 62.61, 62.30, 23.14, 22.14, 13.09, 12.11, 11.07 (m). **IR (neat)**: ν 3060, 2978, 2940, 2879, 1581, 1447, 1214, 1109, 1087, 956, 847, 762, 740, 710, 690 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{11}H_{15}F_3NOS_2$ 298.0542; Found 298.0541. Mp = 37.0 – 37.6 °C.



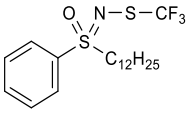
N-trifluoromethylthio-*S*-(4-chlorophenyl)-*S*-2-(methylbut-1-ene) sulfoximine (**2o**). Colorless oil (57%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.77 (dd, *J* = 8.7, 1.3 Hz, 2H), 7.56 (dd, *J* = 8.1, 1.3 Hz, 2H), 5.11 – 5.03 (m, 1H), 4.80 – 4.56 (m, 1H), 4.19 – 4.14 (m, 1H), 3.96 – 3.88 (m, 1H), 1.85 – 1.80 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.13. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 141.24, 134.28, 132.74, 130.90, 130.43 (C-F, $^{1}J_{C\text{-}F}$ = 312.1 Hz), 129.84, 122.62, 63.89, 22.86. **IR (neat)**: ν 3090, 2982, 2923, 1574, 1475, 1447, 1395, 1228, 1109, 1082, 1014, 962, 914, 885, 825, 780, 744, 705, 674 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{11}H_{12}ClF_3NOS_2$ 329.9995; Found 329.9995.



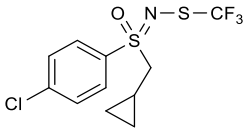
N-trifluoromethylthio-S-benzyl-S-methyl-sulfoximine (**2p**). White solid (81%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.49 – 7.36 (m, 5H), 4.56 (d, *J* = 14.1 Hz, 1H), 4.40 (d, *J* = 14.1 Hz, 1H), 2.88 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.76. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 130.98, 130.57 (C-F, $^{1}J_{C\text{-}F}$ = 312.7 Hz), 129.81, 129.33, 60.58, 37.47. **IR (neat)**: ν 3019, 2924, 1496, 1457, 1411, 1312, 1203, 1150, 1103, 988, 934, 877, 780, 751, 740, 696 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_9H_{11}F_3NOS_2$ 270.0229; Found 270.0229. Mp = 78.0 – 78.7 °C.



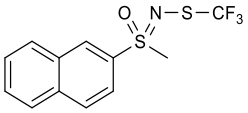
N-trifluoromethylthio-*S*-(4-chlorophenyl)-*S*-benzyl-sulfoximine (**2q**). White solid (61%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.53 – 7.46 (m, 2H), 7.46 – 7.41 (m, 2H), 7.38 – 7.30 (m, 1H), 7.29 – 7.21 (m, 2H), 7.07 – 6.97 (m, 2H), 4.68 (d, *J* = 13.9 Hz, 1H), 4.49 (d, *J* = 13.9 Hz, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.09. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 141.27, 133.65, 131.28, 130.99, 130.44 (C-F, $^{1}J_{C\text{-}F}$ = 312.6 Hz), 129.65, 129.55, 128.89, 126.97, 62.42. **IR (neat)**: ν 3063, 2986, 2928, 1572, 1495, 1472, 1456, 1403, 1394, 1219, 1157, 1106, 1079, 1017, 970, 918, 881, 826, 781, 749, 691 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{14}H_{12}ClF_3NOS_2$ 365.9995; Found 365.9992. Mp = 102.6 – 103.8 °C.



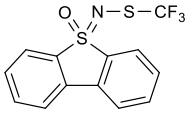
N-trifluoromethylthio-*S*-phenyl-*S*-dodecyl-sulfoximine (**2s**). White semi solid (66%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.89 – 7.80 (m, 2H), 7.72 – 7.66 (m, 1H), 7.65 – 7.56 (m, 2H), 3.51 – 3.38 (m, 1H), 3.33 – 3.15 (m, 1H), 1.90 – 1.73 (m, 1H), 1.64 – 1.49 (m, 2H), 1.40 – 1.13 (m, 18H), 0.87 (t, *J* = 6.9 Hz, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.22. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 136.57, 134.06, 131.64, 129.62, 128.88, 55.83, 31.89, 29.56, 29.53, 29.41, 29.31, 29.18, 28.91, 28.06, 22.68, 22.55, 14.12. **IR (neat)**: ν 2924, 2854, 1466, 1447, 1223, 1149, 1112, 1089, 966, 785, 748, 726, 686 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{19}H_{31}ClF_3NOS_2$ 410.1794; Found 410.1789.



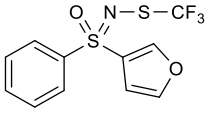
N-trifluoromethylthio-*S*-(4-chlorophenyl)-*S*-methylcyclopropane-sulfoximine (**2t**). Yellow oil (57%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.89 – 7.76 (m, 2H), 7.64 – 7.50 (m, 2H), 3.32 (ddd, *J* = 93.9, 14.6, 7.3 Hz, 2H), 1.04 – 0.90 (m, 1H), 0.67 – 0.59 (m, 1H), 0.57 – 0.44 (m, 1H), 0.32 – 0.21 (m, 1H), 0.06 – 0.00 (m, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.12. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 141.22, 135.14, 130.84, 130.45 (C-F, $^{1}J_{C\text{-}F}$ = 312.7 Hz), 129.96, 61.37, 4.87, 4.84, 4.55. **IR (neat)**: ν 3089, 3014, 1574, 1474, 1395, 1231, 1212, 1082, 1027, 961, 915, 873, 829, 796, 764, 705, 689 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{11}H_{12}F_3NOS_2$ 329.9995; Found 329.9993.



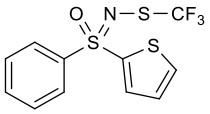
N-trifluoromethylthio-*S*-naphthalene-*S*-methyl sulfoximine (**2v**). White solid (92%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.56 – 8.52 (m, 1H), 8.08 – 8.00 (m, 2H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.80 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.75 – 7.64 (m, 2H), 3.35 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.16. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 135.60, 134.64, 132.41, 130.87, 130.58 (C-F, $^{1}J_{C\text{-}F}$ = 312.3 Hz), 130.28, 129.91, 128.21, 122.42, 43.81. **IR (neat)**: ν 3056, 3023, 2928, 1710, 1625, 1589, 1504, 1404, 1350, 1316, 1272, 1213, 1106, 1068, 984, 954, 938, 869, 857, 818, 764, 750, 708, 632 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{12}H_{11}F_3NOS_2$ 306.0229; Found 306.0227. Mp = 54.5 – 55.7 °C.



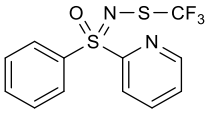
N-trifluoromethylthio-dibenzo[b,d]thiophene sulfoximine (**2w**). White solid (86 %). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 7.7 Hz, 2H), 7.83 (d, *J* = 7.7 Hz, 2H), 7.69 (td, *J* = 7.6, 1.1 Hz, 2H), 7.56 (td, *J* = 7.6, 1.0 Hz, 2H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −50.93. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 136.84, 134.47, 132.73, 130.46, 130.36(C-F, $^{1}J_{C\text{-}F}$ = 312.9 Hz), 124.06, 121.85. **IR (neat)**: ν 3090, 3066, 1590, 1446, 1289, 1279, 1232, 1107, 1062, 971, 772, 755, 738, 721, 709, 675, 613 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{13}H_9F_3NOS_2$ 317.0072; Found 317.0072. Mp = 92.2 – 92.9 °C.



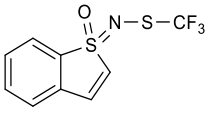
N-trifluoromethylthio-*S*-(3-furyl)-*S*-phenyl-sulfoximine (**2x**). Yellow semi solid (60%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.09 – 8.04 (m, 1H), 8.00 – 7.92 (m, 2H), 7.69 – 7.63 (m, 1H), 7.60 – 7.54 (m, 2H), 7.52 – 7.48 (m, 1H), 6.60 – 6.55 (m, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −50.98. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 147.89, 145.47, 138.95, 134.06, 130.39 (C-F, $^{1}J_{C\text{-}F}$ = 312.1 Hz), 129.68, 128.27, 126.61, 109.10. **IR (neat)**: ν 3147, 3068, 1583, 1543, 1497, 1447, 1238, 1209, 1107, 1007, 975, 935, 870, 818, 718, 683, 625 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{11}H_9F_3NO_2S_2$ 308.0021; Found 308.0020.



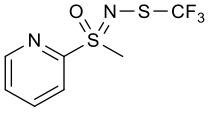
N-trifluoromethylthio-S-(2-thienyl)-S-phenyl-sulfoximine(**2y**). Yellow solid (73%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.05 – 7.96 (m, 2H), 7.74 (dd, *J* = 5.0, 1.4 Hz, 1H), 7.66 (dd, *J* = 3.9, 1.4 Hz, 1H), 7.65 – 7.58 (m, 1H), 7.59 – 7.47 (m, 2H), 7.17 – 7.09 (m, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −50.88. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 139.84, 139.75, 135.66, 134.98, 133.89, 130.37 (C-F, $^1J_{C\text{-}F}$ = 312.5 Hz), 129.66, 128.49, 128.26. **IR (neat)**: ν 3104, 1579, 1502, 1474, 1446, 1396, 1341, 1218, 1160, 1107, 960, 855, 711, 679 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{11}H_9F_3NOS_3$ 323.9793; Found 323.979. Mp = 63.9 – 64.7 °C.



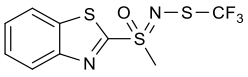
N-trifluoromethylthio-*S*-(2-pyridyl)-*S*-phenyl-sulfoximine (**2z**). White solid (87%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.68 (ddd, *J* = 4.7, 1.8, 0.9 Hz, 1H), 8.39 – 8.27 (m, 1H), 8.22 – 8.07 (m, 2H), 7.96 (td, *J* = 7.8, 1.8 Hz, 1H), 7.71 – 7.61 (m, 1H), 7.60 – 7.53 (m, 2H), 7.48 (ddd, *J* = 7.6, 4.7, 1.1 Hz, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.05. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 156.97, 150.66, 138.26, 136.50, 134.33, 130.49 (C-F, $^1J_{C\text{-}F}$ = 312.6 Hz), 129.93, 129.32, 127.18, 124.52. **IR (neat)**: ν 3082, 1744, 1579, 1475, 1446, 1422, 1295, 1223, 1154, 1108, 1082, 1002, 964, 785, 762, 741, 732, 695, 679, 615 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{12}H_{10}F_3N_2OS_2$ 319.0181; Found 319.0183. Mp = 79.5 – 79.9 °C.



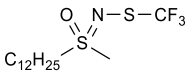
N-trifluoromethylthio-*S*-(benzo[*b*]thiophenyl) sulfoximine (**2aa**). White solid (34%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.87 – 7.82 (m, 1H), 7.63 (td, *J* = 7.5, 1.2 Hz, 1H), 7.57 (td, *J* = 7.6, 1.2 Hz, 1H), 7.46 – 7.41 (m, 1H), 7.31 (d, *J* = 6.8 Hz, 1H), 6.96 (d, *J* = 6.8 Hz, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.41. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 135.88, 134.48, 133.68, 132.77, 131.04, 130.40 (C-F, $^1J_{C\text{-}F}$ = 312.9 Hz), 129.87, 125.81, 123.59. **IR (neat)**: ν 3117, 3093, 1546, 1460, 1337, 1295, 1267, 1215, 1154, 1107, 1077, 964, 862, 787, 757, 717, 676, 610 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_9H_7F_3NOS_2$; 265.9916 Found 265.9913. Mp = 35.5 – 37.5 °C.



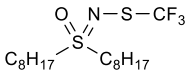
N-(trifluoromethylthio)-*S*-(2-pyridyl)-*S*-methyl sulfoximine (**2ab**). Colorless oil (83%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.79 – 8.73 (m, 1H), 8.21 – 8.14 (m, 1H), 8.04 – 7.98 (m, 1H), 7.61 – 7.55 (m, 1H), 3.46 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.45. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 155.87, 150.40, 138.08, 130.28 (C-F, $^1J_{C\text{-}F}$ = 313.2 Hz), 127.60, 123.60, 39.62. **IR (neat)**: ν 3019, 2931, 1579, 1562, 1453, 1427, 1316, 1222, 1104, 983, 958, 787, 760, 729, 688, 614 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_7H_8F_3N_2OS_2$ 257.0025; Found 257.0025.



N-trifluoromethylthio-*S*-(benzo[*d*]thiazolyl)-*S*-methyl sulfoximine (**2ac**). Orange solid (47%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.26 – 8.17 (m, 1H), 8.09 – 7.97 (m, 1H), 7.70 – 7.58 (m, 2H), 3.62 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.09. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 164.65, 152.68, 137.64, 130.14 (C-F, $^{1}J_{C\text{-}F}$ = 312.1 Hz), 128.37, 127.98, 125.63, 122.46, 42.41. **IR (neat)**: ν 3030, 2999, 2917, 1552, 1468, 1417, 1316, 1227, 1138, 1105, 1026, 986, 966, 851, 761, 729, 706, 689 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_9H_8F_3N_2OS_3$ 312.9745; Found 312.9743. Mp = 88.7 – 90.0 °C.



N-trifluoromethylthio-*S*-dodecyl-*S*-methyl sulfoximine (**2ad**). White solid (92%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 3.35 – 3.14 (m, 2H), 3.07 (s, 3H), 1.85 (dqt, *J* = 11.6, 8.5, 5.7 Hz, 2H), 1.51 – 1.41 (m, 2H), 1.39 – 1.12 (m, 16H), 0.88 (t, *J* = 6.9 Hz, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.78. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 130.59 (C-F, $^{1}J_{C\text{-}F}$ = 312.4 Hz), 54.26, 38.46, 32.03, 29.71, 29.69, 29.58, 29.45, 29.36, 29.12, 28.38, 23.14, 22.82, 14.25. **IR (neat)**: ν 2953, 2919, 2851, 1469, 1418, 1206, 1150, 1105, 1033, 975, 946, 769, 722, 666 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{14}H_{29}F_3NOS_2$ 348.1637; Found 348.1638. Mp = 36.1 – 36.4 °C.

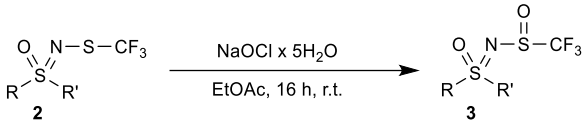


N-trifluoromethylthio-*S*,*S*-dioctyl sulfoximine (**2ae**). Colorless oil (64%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 3.50 – 2.72 (m, 4H), 1.89 – 1.70 (m, 4H), 1.50 – 1.38 (m, 4H), 1.37 – 1.20 (m, 16H), 0.88 (t, *J* = 6.7 Hz, 6H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −51.99. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 130.61 (C-F, $^{1}J_{C\text{-}F}$ = 312.3 Hz), 51.66, 31.80, 29.10, 29.04, 28.50, 22.81, 22.71, 14.17. **IR (neat)**: ν 2925, 2857, 1465, 1406, 1208, 1150, 1110, 971, 751, 723 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{17}H_{35}F_3NOS_2$ 390.2107; Found 390.2109.

References:

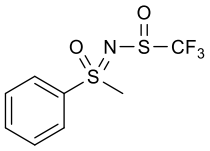
1) C. Bohnen and C. Bolm, *Org. Lett.*, 2015, **17**, 3011–3013.

Preparation of *N*-trifluoromethylsulfaneylidene sulfoximines 3

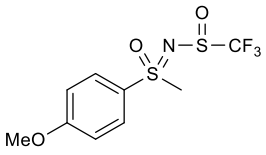


A round bottom flask was charged with trifluoromethylthio sulfoximine **2** (0.3 mmol), EtOAc (1 mL) and NaOCl·5H_2O (1.1 equiv.). The reaction mixture was stirred for 16 h at room temperature. Water was added to the reaction mixture and the product was extracted twice with EtOAc. The organic phase was dried under anhydrous Na_2SO_4 and then evaporated under reduced pressure.

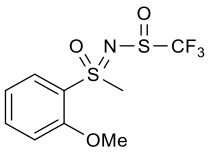
Characterization of *N*-trifluoromethylsulfaneylidene sulfoximines 3



N-(trifluoromethylsulfaneylidene)-*S*-phenyl-*S*-methyl sulfoximine (**3a**). **2a** (0.3 mmol; 86 mg), 1.1 equiv. of NaOCl·5H_2O (0.3 mmol, 49 mg): Colorless oil (92%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.09 – 7.97 (m, 2H), 7.79 – 7.62 (m, 3H), 3.47 – 3.36 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.54, −80.89. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 138.39, 137.83, 135.21, 135.00, 130.23, 130.09, 128.32, 127.54, 124.08 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz), 47.46, 47.16. **IR (neat)**: ν 3067, 3015, 1582, 1448, 1405, 1325, 1231, 1175, 1151, 1090, 1030, 1013, 993, 786, 738, 683 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_9F_3NO_2S_2$ 272.0021; Found 272.0016.

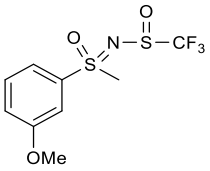


N-(trifluoromethylsulfaneylidene)-*S*-(4-methoxyphenyl)-*S*-methyl sulfoximine (**3b**). **2b** (0.3 mmol; 86 mg), 1.1 equiv. of NaOCl·5H_2O (0.38 mmol, 62 mg): Colorless oil (99%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.00 – 7.87 (m, 2H), 7.13 – 7.04 (m, 2H), 3.91 (s, 3H), 3.47 – 3.27 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.57, −80.94. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 164.99, 164.79, 131.47, 130.78, 129.94, 129.18, 128.36, 124.12 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz), 115.45, 115.27, 56.07, 47.75, 47.50. **IR (neat)**: ν 3017, 2927, 2845, 1593, 1497, 1462, 1444, 1414, 1316, 1265, 1229, 1174, 1151, 1090, 1014, 835, 804, 772, 736, 624 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_9H_{11}F_3NO_3S_2$ 302.0127; Found 302.0126.

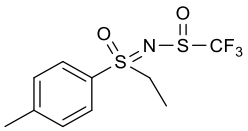


N-(trifluoromethylsulfaneylidene)-*S*-(2-methoxyphenyl)-*S*-methyl sulfoximine (**3c**). **3c** (0.3 mmol; 86 mg), 1.1 equiv. of NaOCl·5H_2O (0.33 mmol, 54 mg): White semi solid (81 mg, 90%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.03 – 7.95 (m, 1H), 7.76 – 7.67 (m, 1H), 7.23 – 7.17 (m, 1H), 7.15 – 7.08 (m, 1H), 4.05 – 3.89 (m, 3H), 3.55 – 3.45 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.87, −81.18. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 157.06, 156.79, 137.43, 137.35, 131.31, 130.72, 124.02 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz), 123.98, 123.70, 121.50 – 121.44 (m), 113.13, 112.64, 56.76, 56.40, 45.00, 44.85. **IR (neat)**: ν 3106, 3027, 2927, 2847, 1591, 1577, 1479, 1435, 1349, 1283, 1254, 1235, 1174, 1151, 1096,

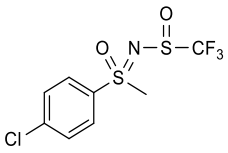
1067, 1043, 1008, 846, 801, 751, 669, 639, 623 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_{11}F_3NO_3S_2$ 302.0127; Found 302.0127.



N-(trifluoromethylsulfaneylidene)-*S*-(3-methoxyphenyl)-*S*-methyl sulfoximine (**3d**). **2d** (0.3 mmol; 86 mg), 1.1 equiv. of $NaOCl{\cdot}5H_2O$ (0.33 mmol, 54 mg): Colorless oil (86 mg, 95%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.64 – 7.43 (m, 3H), 7.28 – 7.21 (m, 1H), 3.92 – 3.84 (m, 3H), 3.46 – 3.34 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.49, −80.91. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 160.67, 160.58, 139.47, 138.74, 131.29, 131.17, 124.09 ((C-F, $^1J_{C\text{-}F}$ = 333.8 Hz), 121.88, 121.41, 120.35, 120.11, 119.52, 112.62, 112.00, 56.05, 55.97, 47.40, 47.05. **IR (neat)**: ν 3077, 3014, 2926, 2842, 1597, 1579, 1484, 1432, 1324, 1290, 1237, 1176, 1151, 1096, 1012, 977, 915, 853, 769, 729, 677 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_{11}F_3NO_3S_2$ 302.0127; Found 302.0126.



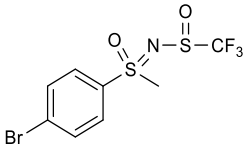
N-(trifluoromethylsulfaneylidene)-*S*-tolyl-*S*-ethyl sulfoximine (**3e**). **2e** (0.3 mmol; 90 mg), 1.1 equiv. of $NaOCl{\cdot}5H_2O$ (0.33 mmol, 54 mg): Colorless oil (69 mg, 77%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.93 – 7.77 (m, 2H), 7.49 – 7.36 (m, 2H), 3.58 – 3.26 (m, 2H), 2.48 (s, 3H), 1.43 – 1.24 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.60, −81.04. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 146.59, 146.30, 133.14, 132.79, 130.76, 130.58, 129.14, 128.30, 124.16 (C-F, $^1J_{C\text{-}F}$ = 333.9 Hz), 54.02, 53.53, 21.84, 21.82, 7.23, 6.83. **IR (neat)**: ν 2980, 2934, 1594, 1493, 1453, 1404, 1383, 1245, 1174, 1152, 1091, 1025, 1003, 916, 814, 776, 726, 694, 632 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{10}H_{13}F_3NO_2S_2$ 300.0334; Found 300.0337.



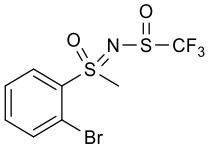
N-(trifluoromethylsulfaneylidene)-*S*-(4-chlorophenyl)-*S*-methyl sulfoximine (**3f**). **2f** (0.3 mmol; 87 mg), 1.1 equiv. of $NaOCl{\cdot}5H_2O$ (0.33 mmol, 54 mg): White semi solid (74 mg, 81%). **IR (neat)**: ν 3092, 3068, 3027, 2928, 1574, 1471, 1396, 1328, 1238, 1173, 1150, 1084, 1018, 1000, 968, 826, 784, 755, 731 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_8H_8ClF_3NO_2S_2$ 305.9632; Found 305.9632.

1. Diasteroisomer (**3f-1**): White solid. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.08 – 7.96 (m, 2H), 7.67 – 7.60 (m, 2H), 3.37 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.77. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 142.32, 136.47, 130.56, 129.85, 124.00 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz), 47.28. Mp = 92.3 – 94.3 °C.

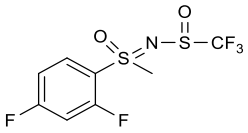
2. Diasteroisomer (**3f-2**): Colorless oil. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.96 – 7.89 (m, 2H), 7.66 – 7.59 (m, 2H), 3.43 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.48. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 142.08, 136.88, 130.45, 129.06, 124.04 (C-F, $^1J_{C\text{-}F}$ = 333.9 Hz), 47.56.



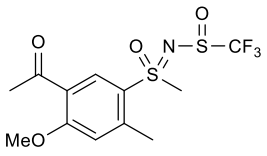
N-(trifluoromethylsulfaneylidene)-*S*-(4-bromophenyl)-*S*-methyl sulfoximine (**3g**). **2g** (0.3 mmol; 100 mg), 1.1 equiv. of NaOCl·5H_2O (0.38 mmol, 62 mg): Colorless oil (102 mg, 97%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.95 – 7.83 (m, 2H), 7.82 – 7.77 (m, 2H), 3.50 – 3.33 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.46, −80.76. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 137.44, 137.02, 133.55, 130.95, 130.68, 129.82, 129.05, 124.02 (C-F, $^1J_{C\text{-}F}$ = 334.1 Hz), 47.50, 47.20. **IR (neat)**: ν 3089, 3016, 2925, 1571, 1470, 1390, 1324, 1233, 1175, 1152, 1089, 1067, 1025, 1000, 824, 775, 740, 712, 622. (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_8BrF_3NO_2S_2$ 349.9126; Found 349.9124.



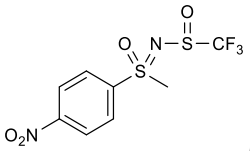
N-(trifluoromethylsulfaneylidene)-*S*-(2-bromophenyl)-*S*-methyl sulfoximine (**3h**). **2h** (0.3 mmol; 100 mg), 1.1 equiv. of NaOCl·5H_2O (0.33 mmol, 54 mg): Colorless oil (78 mg, 74%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.36 – 8.27 (m, 1H), 7.87 – 7.82 (m, 1H), 7.68 – 7.54 (m, 2H), 3.70 – 3.54 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.99, −80.76. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 137.77, 137.29, 136.43, 136.35, 136.03, 135.98, 132.53, 131.86, 128.78, 128.72, 124.03 (C-F, $^1J_{C\text{-}F}$ = 334.8 Hz) 120.70, 120.52, 45.14, 44.71. **IR (neat)**: ν 3089, 3009, 2928, 2251, 1571, 1446, 1428, 1404, 1320, 1233, 1178, 1152, 1098, 1040, 1007, 960, 912, 781, 756, 731, 705, 641 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_8BrF_3NO_2S_2$ 349.9126; Found 349.9127.



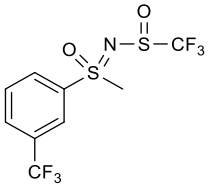
N-(trifluoromethylsulfaneylidene)-*S*-(2,4-difluorophenyl)-*S*-methyl sulfoximine (**3i**). **2i** (0.3 mmol; 87 mg), 1.1 equiv. of NaOCl·5H_2O (0.38 mmol, 62 mg): White semi solid (90 mg, 97%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.21 – 7.96 (m, 1H), 7.21 – 7.02 (m, 2H), 3.68 – 3.37 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.53 – (−80.78) (m), −95.91 (tt, *J* = 14.2, 7.3 Hz), −101.22 – (−102.66) (m). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.14 – 168.17 (m), 167.11 – 166.25 (m), 161.49 – 160.41 (m), 159.04 – 158.11 (m), 133.47 – 132.88 (m), 132.64 – 132.23 (m), 123.90 (C-F, $^1J_{C\text{-}F}$ = 333.9 Hz), 122.43 – 121.90 (m), 113.47 – 113.38 (m), 113.38 – 113.31 (m), 113.32 – 113.19 (m), 113.20 – 113.07 (m), 106.91 – 106.32 (C-F, $^1J_{C\text{-}F}$ = 12.3 Hz), 46.63 – 46.17 (m). **IR (neat)**: ν 3105, 3068, 3044, 2946, 1771, 1599, 1479, 1431, 1396, 1359, 1326, 1279, 1236, 1180, 1151, 1101, 1070, 1028, 971, 886, 859, 822, 779, 739, 727, 696, 620 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_7F_5NO_2S_2$ 307.9833; Found 307.9834.



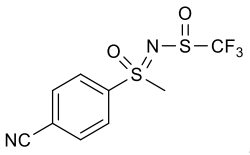
N-(trifluoromethylsulfaneylidene)-*S*-(5-acetyl-4-methoxy-2-methylphenyl)-*S*-methyl sulfoximine (**3j**). **2j** (0.3 mmol; 102 mg), 1.5 equiv. of NaOCl·5H_2O (0.45 mmol, 74 mg): White semi solid (97 mg, 91%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.48 – 8.41 (m, 1H), 6.98 – 6.95 (m, 1H), 4.02 (s, 3H), 3.48 – 3.39 (m, 3H), 2.80 – 2.73 (m, 3H), 2.61 – 2.59 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.32, −80.83. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 197.01, 196.80, 162.89, 162.70, 144.59, 144.32, 133.72, 132.56, 128.58, 128.13, 126.72, 126.59, 124.07 (C-F, $^1J_{C\text{-}F}$ = 334.2 Hz), 116.68, 116.55, 56.55 – 56.44 (m), 46.95, 45.92, 31.80 – 31.65 (m), 29.70, 21.85, 21.19. **IR (neat)**: ν 3005, 2923, 1670, 1595, 1550, 1485, 1468, 1443, 1390, 1264, 1232, 1171, 1150, 1084, 1013, 984, 876, 775, 747, 687, 619 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{12}H_{15}F_3NO_4S_2$ 358.0389; Found 358.0387.



N-(trifluoromethylsulfaneylidene)-*S*-(4-nitrophenyl)-*S*-methyl sulfoximine (**3k**). **2k** (0.3 mmol; 90 mg), 1.1 equiv. of NaOCl·5H_2O (0.33 mmol, 54 mg): Yellow oil (89 mg, 94%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.52 – 8.47 (m, 2H), 8.32 – 8.20 (m, 2H), 3.55 – 3.41 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.31, −80.56. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 151.62, 151.53, 144.27, 129.94, 129.19, 125.25, 123.97 (C-F, $^1J_{C\text{-}F}$ = 334.0 Hz), 47.45, 47.09. **IR (neat)**: ν 3107, 3019, 2927, 1607, 1530, 1402, 1348, 1237, 1177, 1152, 1088, 1025, 1004, 853, 779, 736, 711, 678 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_8F_3N_2O_4S_2$ 316.9872; Found 316.9872.

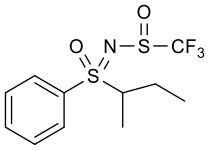


N-(trifluoromethylsulfaneylidene)-*S*-(3-trifluoromethylphenyl)-*S*-methyl sulfoximine (**3l**). **2l** (0.3 mmol; 97 mg), 1.1 equiv. of NaOCl·5H_2O (0.45 mmol, 74 mg): orange oil (79 mg, 78%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.36 – 8.16 (m, 2H), 8.04 – 7.99 (m, 1H), 7.90 – 7.76 (m, 1H), 3.51 – 3.39 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −63.39, −63.45, −80.44, −80.65. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 140.02, 139.78, 133.42 – 132.48 (m), 131.95 – 131.53 (m), 131.11, 131.05, 130.92, 125.61 – 125.43 (m), 124.94 – 124.55 (m), 124.02 (C-F, $^1J_{C\text{-}F}$ = 333.9 Hz), 122, 88(C-F, $^1J_{C\text{-}F}$ = 272.8 Hz), 47.53, 47.24. **IR (neat)**: ν 3017, 2956, 2918, 2849, 1718, 1609, 1433, 1378, 1325, 1282, 1239, 1175, 1135, 1102, 1070, 1024, 995, 909, 806, 771, 731, 692, 649, 625 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_9H_8F_6NO_2S_2$ 339.9895; Found 339.9896.

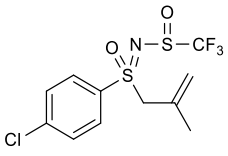


N-(trifluoromethylsulfaneylidene)-*S*-(4-cyanophenyl)-*S*-methyl sulfoximine (**3m**). **2m** (0.3 mmol; 84 mg), 1.2 equiv. of NaOCl·5H_2O (0.36 mmol, 59 mg): Colorless oil (84 mg, 95%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.25 – 8.11 (m, 2H), 8.00 – 7.92 (m, 2H), 3.50 – 3.38 (m, 3H). **^{19}F NMR**

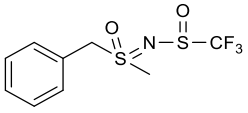
(471 MHz, Chloroform-*d*) δ −80.35, −80.60. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 143.07 – 142.43 (m), 134.06 – 133.29 (m), 129.34 – 128.86 (m), 128.64 – 128.07 (m), 123.98 (C-F, $^{1}J_{C\text{-}F}$ = 334.2 Hz), 118.99, 118.87, 116.97 – 116.32 (m), 47.89 – 47.29 (m), 47.21 – 46.78 (m). **IR (neat)**: ν 3096, 3017, 2925, 2236, 1487, 1399, 1323, 1236, 1176, 1153, 1087, 1028, 1007, 840, 789, 727, 708 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_8F_3N_2O_2S_2$ 296.9974; Found 296.9971.



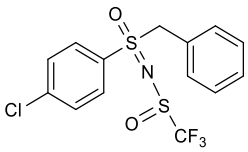
N-(trifluoromethylsulfaneylidene)-*S*-phenyl-*S*-(*sec*-butyl) sulfoximine (**3n**). **2n** (0.3 mmol; 94 mg), 1.1 equiv. of NaOCl·5H$_2$O (0.33 mmol, 54 mg): Colorless oil (91 mg, 97%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.04 – 7.86 (m, 2H), 7.79 – 7.71 (m, 1H), 7.68 – 7.58 (m, 2H), 3.35 – 3.11 (m, 1H), 2.21 – 1.95 (m, 1H), 1.62 – 1.42 (m, 1H), 1.42 – 1.28 (m, 3H), 1.07 – 0.94 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.44 – (−80.60) (m), −80.96 – (−81.12) (m). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 135.52, 135.46 – 135.35 (m), 134.96, 134.76 – 134.68 (m), 124.17 (C-F, $^{1}J_{C\text{-}F}$ = 333.4 Hz), 65.38, 65.16, 64.79, 64.50, 22.21, 22.17, 22.04, 22.01, 12.29, 12.17, 11.98, 11.18, 11.12, 11.10, 11.01. **IR (neat)**: ν 3068, 2979, 2942, 2883, 1582, 1447, 1356, 1174, 1151, 1090, 1031, 1009, 992, 845, 750, 722, 687 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{11}H_{15}F_3NO_2S_2$ 314.0491; Found 314.0492.



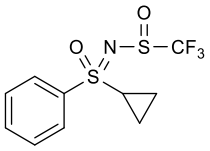
N-(trifluoromethylsulfaneylidene)-*S*-(4-chlorophenyl)-*S*-2-(methylbut-1-ene) sulfoximine (**3o**). **2o** (0.3 mmol; 99 mg), 1.1 equiv. of NaOCl·5H$_2$O (0.45 mmol, 74 mg): Yellowish oil (99 mg, 96%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.99 – 7.79 (m, 2H), 7.63 – 7.51 (m, 2H), 5.24 – 5.11 (m, 1H), 4.88 – 4.65 (m, 1H), 4.26 – 3.97 (m, 2H), 1.91 – 1.75 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.50, −80.72. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 142.15, 141.94, 134.67, 134.39, 131.69, 131.38, 130.81, 130.15 – 130.07 (m), 129.99, 124.00 (C-F, $^{1}J_{C\text{-}F}$ = 334.4 Hz), 123.77, 67.49, 66.79, 22.86. **IR (neat)**: ν 3092, 2978, 2921, 1575, 1475, 1395, 1235, 1177, 1152, 1083, 1025, 1002, 918, 889, 827, 785, 755, 723, 705, 673, 619 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{11}H_{12}ClF_3NO_2S_2$ 345.9945; Found 345.9943.



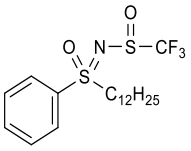
N-(trifluoromethylsulfaneylidene)-*S*-benzyl-*S*-methyl sulfoximine (**3p**). **2p** (0.3 mmol; 81 mg), 1.1 equiv. of NaOCl·5H$_2$O (0.33 mmol, 54 mg): White solid (83 mg, 97%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.51 – 7.38 (m, 5H), 4.68 – 4.51 (m, 2H), 3.17 – 2.94 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.50, −80.77. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 131.51 – 131.05 (m), 130.38, 130.27, 129.59 – 129.43 (m), 126.48, 125.75, 124.04 (C-F, $^{1}J_{C\text{-}F}$ = 334.5 Hz), 64.71, 63.85, 42.19, 40.96. **IR (neat)**: ν 3032, 3014, 2980, 2924, 2254, 1495, 1457, 1406, 1319, 1175, 1149, 1094, 1040, 965, 909, 882, 827, 783, 756, 723, 695, 648 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_{11}F_3NO_2S_2$ 286.0178; Found 286.0177. Mp = 65.4 – 68.9 °C.



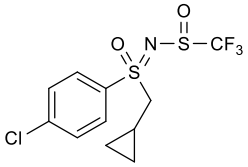
N-(trifluoromethylsulfaneylidene)-*S*-(4-chlorophenyl)-*S*-benzyl sulfoximine (**3q**). **2q** (0.3 mmol; 110 mg), 1.1 equiv. of NaOCl·5H_2O (0.33 mmol, 54 mg): Colorless oil (109 mg, 95%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.69 – 7.51 (m, 2H), 7.51 – 7.43 (m, 2H), 7.41 – 7.35 (m, 1H), 7.33 – 7.27 (m, 2H), 7.13 – 7.05 (m, 2H), 4.74 – 4.54 (m, 2H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.43, −80.66. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 142.20, 141.97, 134.24, 133.72, 131.61 – 131.45 (m), 130.93, 130.20, 130.13, 130.02, 129.98, 129.80, 129.12 – 128.78 (m), 126.00, 125.43, 124.13 (C-F, $^1J_{C\text{-}F}$ = 334.2 Hz) 66.41, 65.53. **IR (neat)**: ν 3091, 3067, 3036, 2978, 2925, 1574, 1495, 1474, 1457, 1395, 1235, 1176, 1153, 1083, 1024, 999, 921, 880, 826, 783, 755, 730, 696, 624, 609. (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{14}H_{12}ClF_3NO_2S_2$ 381.9945; Found 381.9944.



N-(trifluoromethylsulfaneylidene)-*S*-phenyl-*S*-cyclopropyl sulfoximine (**3r**). **2r** (0.3 mmol; 84 mg), 1.1 equiv. of NaOCl·5H_2O (0.33 mmol, 54 mg): Colorless oil (75 mg, 84%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.03 – 7.94 (m, 2H), 7.77 – 7.70 (m, 1H), 7.68 – 7.59 (m, 2H), 2.84 – 2.68 (m, 1H), 1.69 – 1.58 (m, 2H), 1.47 – 1.23 (m, 2H), 1.18 – 1.09 (m, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.75, −80.96. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 138.36, 138.26, 134.80, 134.62, 130.04, 129.90, 128.31, 127.71, 124.10 (C-F, $^1J_{C\text{-}F}$ = 333.5 Hz), 35.34, 35.22, 7.34 – 7.11 (m), 6.91, 6.30. **IR (neat)**: ν 3047, 1477, 1448, 1421, 1310, 1231, 1175, 1152, 1093, 1010, 992, 880, 826, 745, 725, 684 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{10}H_{11}F_3NO_2S_2$ 298.0178; Found 298.0179.

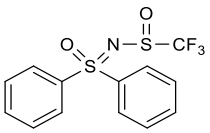


N-(trifluoromethylsulfaneylidene)-*S*-phenyl-*S*-dodecyl sulfoximine (**3s**). **2s** (0.3 mmol; 123 mg), 1.1 equiv. of NaOCl·5H_2O (0.33 mmol, 54 mg): White semi solid (126 mg, 98%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.06 – 7.91 (m, 2H), 7.80 – 7.60 (m, 3H), 3.53 – 3.26 (m, 2H), 1.96 – 1.60 (m, 2H), 1.43 – 1.12 (m, 18H), 0.92 – 0.79 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.55, −80.98. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 137.05, 136.85, 135.05, 134.82, 130.11, 129.95, 128.96, 128.15, 124.17 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz), 59.25, 58.76, 32.02, 29.73 – 29.64 (m), 29.53, 29.44, 29.35 – 29.22 (m), 29.10 – 28.91 (m), 22.81, 22.32, 21.95, 14.25. **IR (neat)**: ν 2924, 2854, 1466, 1448, 1402, 1377, 1228, 1177, 1154, 1092, 1032, 1015, 994, 788, 746, 685 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{19}H_{31}F_3NO_2S_2$ 426.1743; Found 426.174.

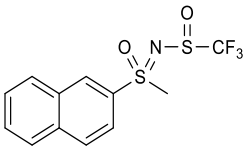


N-(trifluoromethylsulfaneylidene)-*S*-(4-chlorophenyl)-*S*-cyclopropylmethyl sulfoximine (**3t**). **2t** (0.3 mmol; 99 mg), 1.1 equiv. of NaOCl·5H_2O (0.33 mmol, 54 mg): Colorless oil (100 mg, 97%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.05 – 7.88 (m, 2H), 7.67 – 7.50 (m, 2H), 3.53 – 3.24 (m, 2H), 1.12 – 1.00 (m, 1H), 0.73 – 0.55 (m, 2H), 0.37 – 0.23 (m, 1H), 0.21 – 0.11 (m, 1H). **^{19}F NMR** (471

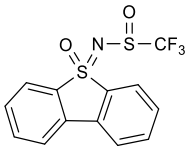
MHz, Chloroform-*d*) δ −80.59, −80.89. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 142.18, 141.96, 135.42, 135.34, 130.78, 130.28, 130.16, 130.01, 124.11 (C-F, $^{1}J_{C\text{-}F}$ = 334.2 Hz), 64.98, 64.38, 4.83, 4.69, 4.64, 4.52, 4.20. **IR (neat)**: ν 3092, 3015, 2969, 2918, 1576, 1474, 1396, 1176, 1152, 1083, 1025, 1002, 915, 876, 830, 798, 766, 719 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{11}H_{12}ClF_3NO_2S_2$ 345.9945; Found 345.994.



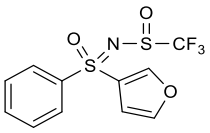
N-(trifluoromethylsulfaneylidene)-*S,S*-diphenyl sulfoximine (**3u**). **2u** (0.3 mmol; 95 mg), 1.1 equiv. of NaOCl·5H$_2$O (0.33 mmol, 54 mg): White solid (82 mg, 82%). Needed column chromatography (EtoAc:hexane) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.10 – 7.94 (m, 4H), 7.70 – 7.63 (m, 2H), 7.62 – 7.51 (m, 4H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.57. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 139.09, 138.91, 134.58, 134.43, 130.06, 129.91, 128.43, 127.93, 124.18 (C-F, $^{1}J_{C\text{-}F}$ = 333.6 Hz). **IR (neat)**: ν 3068, 1475, 1449, 1230, 1153, 1090, 1044, 1018, 993, 858, 762, 725, 681 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{13}H_{11}F_3NO_2S_2$ 334.0178; Found 334.0177. Mp = 76.8 – 77.3 °C.



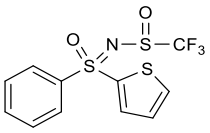
N-(trifluoromethylsulfaneylidene)-*S*-naphthalenyl-*S*-methyl sulfoximine (**3v**). **2v** (0.3 mmol; 92 mg), 1.1 equiv. of NaOCl·5H$_2$O (0.33 mmol, 54 mg): Brown oil (95 mg, 98%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.70 – 8.52 (m, 1H), 8.11 – 8.02 (m, 2H), 8.00 – 7.85 (m, 2H), 7.78 – 7.65 (m, 2H), 3.56 – 3.40 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.46, −80.84. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 135.88, 135.73, 134.88, 134.32, 132.29, 132.19, 130.89, 130.77, 130.63, 130.41, 130.36, 129.93, 129.82, 129.76, 128.53, 128.51, 128.30 – 128.13 (m), 124.13 (C-F, $^{1}J_{C\text{-}F}$ = 333.9 Hz), 122.02, 121.47, 47.31, 47.09. **IR (neat)**: ν 3059, 3018, 2926, 2251, 1748, 1625, 1589, 1504, 1403, 1350, 1321, 1270, 1230, 1177, 1152, 1102, 1071, 1014, 940, 907, 858, 815, 773, 726, 637, 605 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{12}H_{11}F_3NO_2S_2$ 322.0178; Found 322.0176.



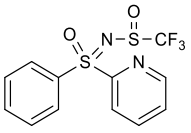
N-(trifluoromethylsulfaneylidene)-dibenzo[b,d]thienyl sulfoximine (**3w**). **2w** (0.3 mmol; 95 mg), 1.1 equiv. of NaOCl·5H$_2$O (0.33 mmol, 54 mg): White solid (90 mg, 91%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.00 – 7.90 (m, 2H), 7.86 – 7.80 (m, 2H), 7.79 – 7.68 (m, 2H), 7.64 – 7.57 (m, 2H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.20. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 137.19, 136.66, 135.55, 135.22, 132.78, 132.30, 131.28, 131.17, 124.10, 123.99, 122.24, 122.18. **IR (neat)**: ν 3088, 3059, 1590, 1481, 1448, 1175, 1151, 1127, 1096, 1068, 1001, 870, 770, 756, 734, 721, 703, 687, 637, 614 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{13}H_9F_3NO_2S_2$ 332.0021; Found 332.0018. Mp = 107.2 – 109.0 °C.



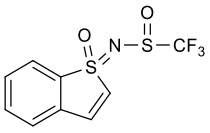
N-(trifluoromethylsulfaneylidene)-*S*-phenyl-*S*-(3-furyl) sulfoximine (**3x**). **2x** (0.3 mmol; 92 mg), 1.1 equiv. of NaOCl·5H_2O (0.33 mmol, 54 mg): Colorless oil (89 mg, 92%). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 8.20 – 8.12 (m, 1H), 8.09 – 8.00 (m, 2H), 7.75 – 7.58 (m, 3H), 7.56 – 7.49 (m, 1H), 6.75 – 6.52 (m, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −80.50, −80.52. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 148.38, 147.76, 146.10, 146.05, 139.02, 138.66, 134.87, 134.67, 130.09, 129.94, 128.07, 127.56, 127.28, 127.00, 124.10 (C-F, $^1J_{C\text{-}F}$ = 333.3 Hz), 108.99, 108.56. **IR (neat)**: ν 3133, 1542, 1497, 1448, 1247, 1178, 1145, 1091, 1009, 994, 941, 870, 821, 726, 682, 626 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{11}H_9F_3NO_3S_2$ 323.997; Found 323.9968.



N-(trifluoromethylsulfaneylidene)-*S*-(phenyl)-*S*-(2-thienyl) sulfoximine (**3y**). **2y** (0.384 mmol; 124 mg), 1.1 equiv. of NaOCl·5H_2O (0.422 mmol, 69 mg): Yellowish oil (123 mg, 97%). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 8.11 – 8.05 (m, 2H), 7.87 – 7.74 (m, 2H), 7.71 – 7.64 (m, 1H), 7.63 – 7.55 (m, 2H), 7.20 – 7.14 (m, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −80.32, −80.42. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 139.98, 139.82, 139.67, 136.63, 136.36, 135.99, 135.10, 134.65, 134.48, 130.03, 129.91, 128.92, 128.73, 128.02, 127.54, 124.18 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz). **IR (neat)**: ν 3094, 1502, 1476, 1447, 1397, 1342, 1240, 1177, 1153, 1089, 1022, 990, 856, 723, 681, 665 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{11}H_9F_3NO_2S_3$ 339.9742; Found 339.9739.

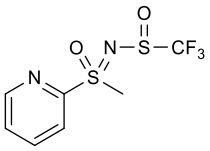


N-(trifluoromethylsulfaneylidene)-*S*-phenyl-*S*-(2-pyridyl) sulfoximine (**3z**). **2z** (0.3 mmol; 95 mg), 1.1 equiv. of NaOCl·5 H_2O (0.33 mmol, 54 mg): Colorless oil (98 mg, 98%). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 8.77 – 8.64 (m, 1H), 8.40 – 8.29 (m, 1H), 8.19 – 8.11 (m, 2H), 8.08 – 7.95 (m, 1H), 7.74 – 7.67 (m, 1H), 7.65 – 7.57 (m, 2H), 7.57 – 7.51 (m, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −80.53, −80.75. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 157.22, 156.93, 150.97 – 150.80 (m), 138.96, 138.79, 136.54, 136.45, 134.97, 134.85, 129.82 – 129.71 (m), 129.65, 129.37, 127.89, 127.79, 124.19 (C-F, $^1J_{C\text{-}F}$ = 334.1 Hz), 123.70, 123.17. **IR (neat)**: ν 3091, 3066, 1578, 1560, 1476, 1448, 1425, 1241, 1177, 1153, 1087, 1031, 1013, 988, 844, 775, 741, 700, 681, 615 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{12}H_{10}F_3N_2O_2S_2$ 335.013; Found 335.0131.

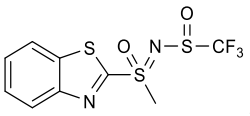


N-(trifluoromethylsulfaneylidene)-*S*-(benzo[*b*]thienyl) sulfoximine (**3aa**). **2aa** (0.3 mmol; 80 mg), 1.5 equiv. of NaOCl·5H_2O (0.45 mmol, 74 mg): Orange semi solid (20 mg, 24%). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 7.94 – 7.85 (m, 1H), 7.70 – 7.60 (m, 2H), 7.52 – 7.46 (m, 1H), 7.42 – 7.35 (m, 1H), 7.07 – 6.98 (m, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −80.09, −80.56. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 136.28, 135.86, 135.09, 134.91, 134.67, 133.73, 132.09, 131.78, 131.74, 131.57, 130.86, 130.58, 126.20 – 126.05 (m), 123.96 (C-F, $^1J_{C\text{-}F}$ = 335.2 Hz), 123.47, 123.35. **IR (neat)**: ν 3065,

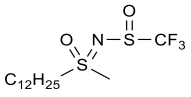
1548, 1460, 1369, 1340, 1297, 1272, 1245, 1149, 1085, 1051, 1011, 876, 792, 758, 698, 682, 628 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_7F_3NO_2S_2$ 281.9865; Found 281.9867.



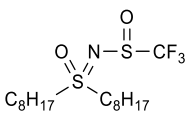
N-(trifluoromethylsulfaneylidene)-*S*-(2-pyridyl)-*S*-methyl sulfoximine (**3ab**). **2ab** (0.3 mmol; 77 mg), 1.1 equiv. of $NaOCl{\cdot}5H_2O$ (0.33 mmol, 54 mg): Colorless oil (72 mg, 88%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.83 – 8.75 (m, 1H), 8.32 – 8.16 (m, 1H), 8.11 – 8.04 (m, 1H), 7.71 – 7.63 (m, 1H), 3.62 – 3.53 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.63 – (−80.75) (m), −80.77 – (−81.08) (m). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 156.26 – 155.78 (m), 150.59, 150.52, 139.06, 138.93, 128.42 (m), 123.90 (C-F, $^1J_{C\text{-}F}$ = 334.7 Hz), 122.67, 122.04, 42.51, 42.46. **IR (neat)**: ν 3087, 3016, 2927, 1580, 1561, 1453, 1428, 1405, 1317, 1234, 1176, 1152, 1102, 1016, 988, 790, 762, 737, 703, 614 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_7H_8F_3N_2O_2S_2$ 272.9974; Found 272.9974.



N-(trifluoromethylsulfaneylidene)-*S*-(benzo[*d*]thiazol-2-yl)-*S*-methyl sulfoximine (**3ac**). **2ac** (0.3 mmol; 94 mg), 1.1 equiv. of $NaOCl{\cdot}5H_2O$ (0.33 mmol, 54 mg): Orange semi solid (81 mg, 82%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.28 – 8.18 (m, 1H), 8.09 – 7.99 (m, 1H), 7.76 – 7.56 (m, 2H), 3.79 – 3.68 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.28, −80.40. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 164.51, 164.16, 152.61, 137.71, 137.50, 128.91, 128.30, 125.94, 125.80, 123.93 (C-F, $^1J_{C\text{-}F}$ = 334.8 Hz), 122.56, 122.54, 45.51, 45.16. **IR (neat)**: ν 3012, 2921, 1553, 1466, 1417, 1316, 1242, 1179, 1153, 1098, 1046, 1008, 958, 851, 760, 726, 684, 606 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_8F_3N_2O_2S_3$ 328.9695; Found 328.9694.



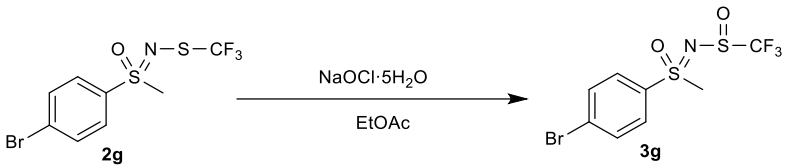
N-(trifluoromethylsulfaneylidene)-*S*-dodecyl-*S*-methyl sulfoximine (**3ad**). **2ad** (0.3 mmol; 104 mg), 1.1 equiv. of $NaOCl{\cdot}5H_2O$ (0.33 mmol, 54 mg): White solid (107 mg, 98%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 3.37 – 3.18 (m, 5H), 1.97 – 1.85 (m, 2H), 1.52 – 1.42 (m, 2H), 1.40 – 1.16 (m, 17H), 0.88 (t, *J* = 6.9 Hz, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.79 – (−80.83) (m). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 124.03 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz) 57.94, 57.25, 43.70, 42.98, 32.03, 29.71, 29.68, 29.62 – 29.52 (m), 29.45, 29.35, 29.31, 29.07, 28.20, 28.12, 22.82, 22.43, 21.86, 14.26. **IR (neat)**: ν 3013, 2919, 2851, 1468, 1414, 1322, 1216, 1170, 1152, 1092, 1021, 967, 884, 837, 780, 747, 719, 702, 665 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{29}F_3NO_2S_2$ 364.1586; Found 364.1583. Mp = 53.0 – 54.7 °C.



N-(trifluoromethylsulfaneylidene)-*S,S*-dioctyl sulfoximine (**3ae**). **2ae** (0.3 mmol; 125 mg), 1.1 equiv. of $NaOCl{\cdot}5H_2O$ (0.33 mmol, 54 mg): Yellow oil (123 mg, 95%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 3.32 – 3.11 (m, 4H), 1.99 – 1.81 (m, 4H), 1.51 – 1.40 (m, 4H), 1.38 – 1.19 (m, 16H), 0.93

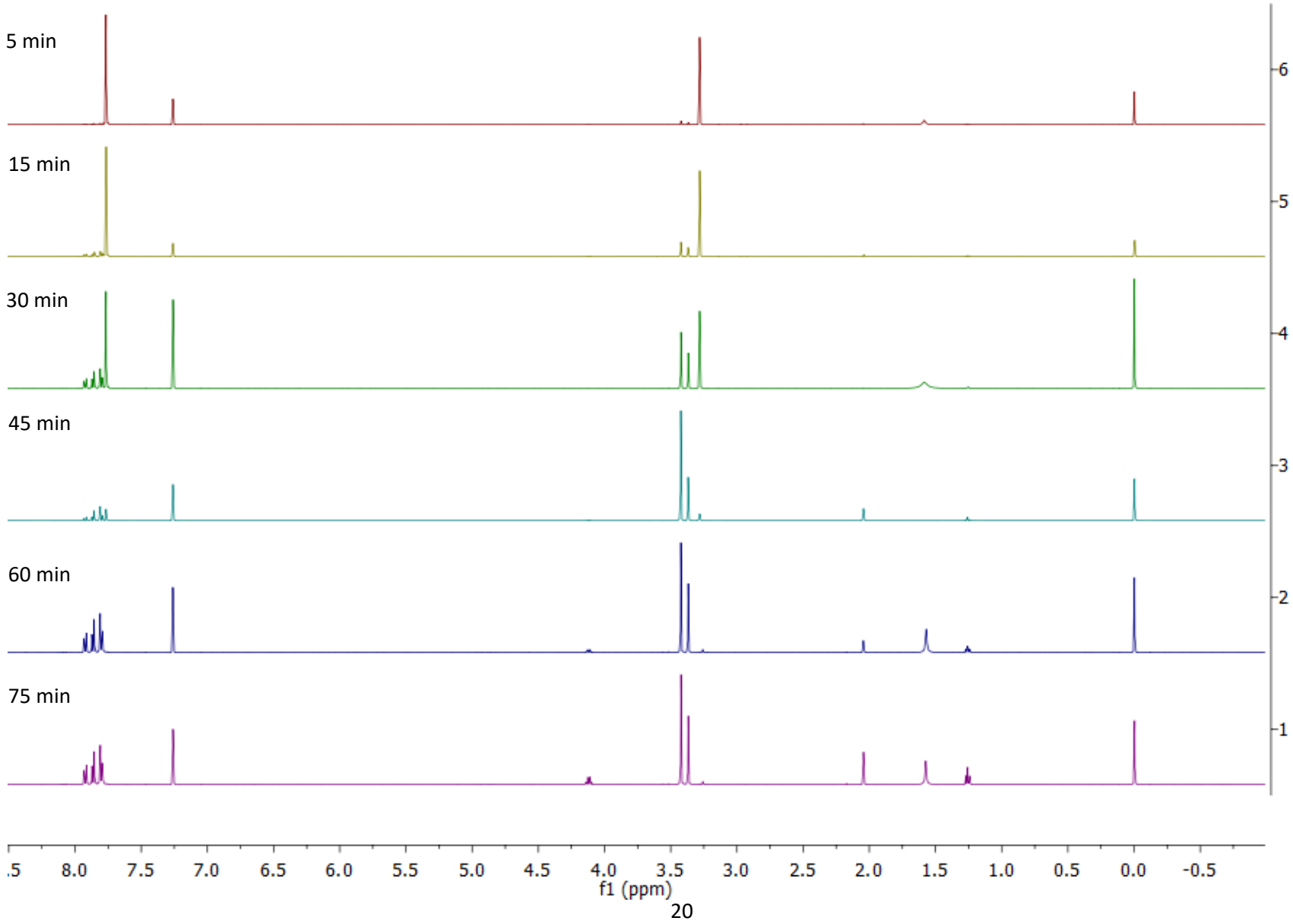
– 0.82 (m, 6H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.75. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 124.15 (C-F, $^{1}J_{C\text{-}F}$ = 333.7 Hz), 56.04, 54.84, 31.82 – 31.69 (m), 29.10 – 28.87 (m), 28.32, 28.22, 22.70, 21.80, 21.25, 14.57 – 13.89 (m). **IR (neat)**: ν 2955, 2926, 2857, 1465, 1404, 1379, 1176, 1151, 1102, 1022, 746, 722 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{17}H_{35}F_3NO_2S_2$ 406.2056; Found 406.2053.

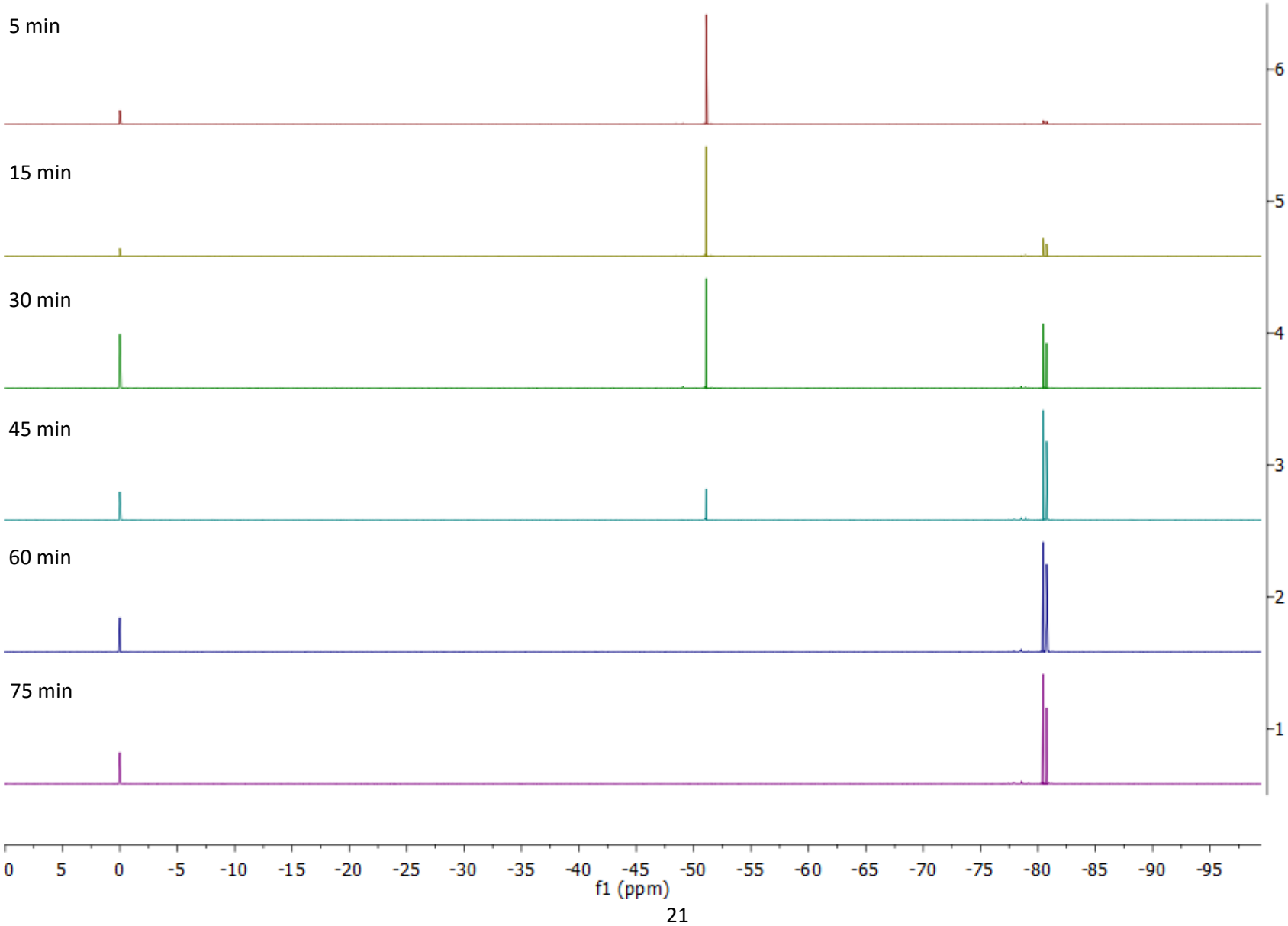
Gram-scale reaction



A round bottom flask was charged with *N*-(trifluoromethylthio)-*S*-(4-bromophenyl)-*S*-methyl sulfoximine (**2g**) (1.00 g, 3.0 mmol), EtOAc (4 mL) and $NaOCl{\cdot}5H_2O$ (1.25 equiv.). After 5 minutes of stirring, an aliquot (cca. 0.1 mL) was taken. The solvent was removed under reduced pressure and the residue was analysed with ^{1}H NMR and ^{19}F NMR. An aliquot was subsequently taken every 15 min. After completion water was added to the reaction mixture and the product was extracted twice with EtOAc. The organic phase was dried under anhydrous Na_2SO_4 and then evaporated under reduced pressure yielding 1.02 g (97%) of **3g**.

The ^{1}H and ^{19}F NMR spectra after 5, 15, 30, 45, 60 and 75 min are provided in descending order. The starting substrate **2g** was no longer observable between the 45- and 60-min interval.


5 min
15 min
30 min
45 min
60 min
75 min
6
5
4
3
2
1
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


5 min
15 min
30 min
45 min
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75 min
6
5
4
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2
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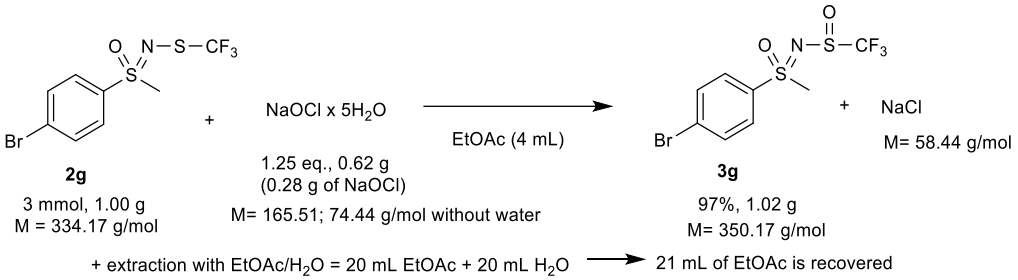
0 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95
f1 (ppm)

Green chemistry metrics



Atom economy: (M of desired product / M of all reactants) x 100 = 350.17 / (334.17 + 74.44 x 1.25) = **82.0%**

Actual atom economy: (% yield of product · % atom economy) x 100 = 97% · 82.0% = **79.5%**

Reaction mass efficiency: (Mass of product / mass of all reagents) · 100 = 1.02 / (1.00 + 0.28) = **79.7%**

E-factor: (Amount of waste / amount of product) = (16.81 g) / 1.02 g = **16.48**

Amount of reactants: 1.00 g + 0.62 g = 1.62 g

Amount of waste from reaction: 1.62 − 1.02 = 0.60 g

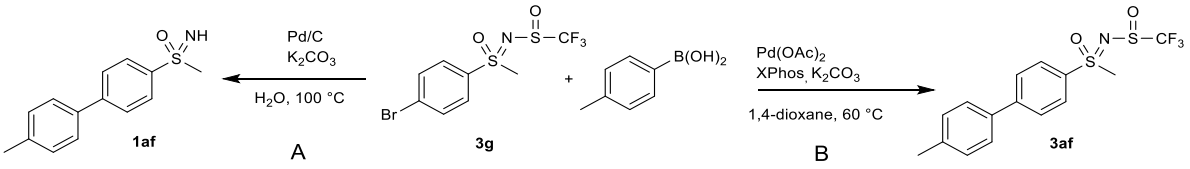
Amount of waste from purification: 3 mL of **EtOAc** (d = 0.902 g/mL) = 2.71 g; 10 g of **water**; 3.5 g of **Na_2SO_4**.

Amount of waste: 0.60 g + 2.71 g + 10 g + 3.5 g = 16.81 g

EcoScale: Points deducted for yield (−1.5), $NaOCl{\cdot}5H_2O$ is classified as dangerous for the environment (−5), EtOAC is flammable (−5), time of reaction (−1) and liquid-liquid extraction (−3). Final score: 84.5.

Post-modification reactions

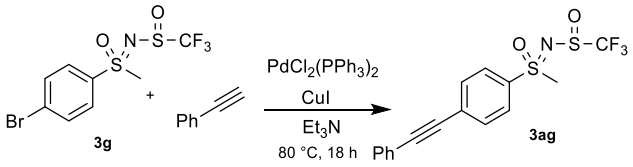
Suzuki-Miyaura reaction



Procedure A: A round bottom flask was charged with *N*-(trifluoromethylsulfaneylidene)-*S*-(4-bromophenyl)-*S*-methyl sulfoximine (**3g**) (33 mg, 0.1 mmol), 4-methylphenyl boronic acid (1.33 equiv.) and K_2CO_3 (3 equiv.). Water (3 mL) was added followed by palladium on carbon (tip of the spatula) and the reaction mixture was stirred for 1 h under reflux. After 1 h, the reaction mixture was cooled to room temperature and extracted with EtOAc. The solvent was removed under reduced pressure and the residue was purified by column chromatography yielding **1af** (22 mg, 90%).

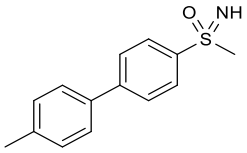
Procedure B: A Schlenk tube was charged with *N*-(trifluoromethylsulfaneylidene)-*S*-(4-bromophenyl)-*S*-methyl sulfoximine (**3g**) (67 mg, 0.2 mmol), 4-methylphenyl boronic acid (1.1 equiv.), $Pd(OAc)_2$ (10 mol%) and XPhos (10 mol%). The tube was equipped with a septum and an argon balloon. The mixture was stirred for 10 min at room temperature, then a 2 M aqueous degassed K_2CO_3 solution (0.5 mL, 5.0 equiv.) was added with a syringe and the mixture was heated at 60 °C for 24 h. The mixture was cooled to room temperature. The solvents were removed under reduced pressure and the residue was purified by column chromatography furnishing **3af** (54 mg, 75%).

Sonogashira reaction

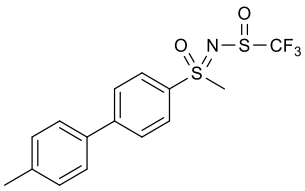


A dried round bottom flask was charged with *N*-(trifluoromethylsulfaneylidene)-*S*-(4-bromophenyl)-*S*-methyl sulfoximine (**3g**) (0.11 g, 0.3 mmol) and Et_3N (3 mL). The flask was equipped with a septum and an argon balloon. To this solution $PdCl_2(PPh_3)_2$ (21 mg, 10 mol%) and CuI (6 mg, 10 mol%) were added and the reaction mixture was stirred for 5 min under an inert atmosphere, followed by the addition of phenylacetylene (50 µL, 0.45 mmol, 1.5 equiv.). The resulting mixture was then heated to 80 °C for 18 h under an inert atmosphere. The mixture was cooled to room temperature and the solvent was removed under reduced pressure. The crude reaction mixture was extracted with ethyl acetate (3 x 10 mL). The combined organic layer was washed with brine (30 mL), dried over anhydrous sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography and both diastereoisomers of **3ag** were isolated (76 mg, 68%).

Characterization of post-modification products



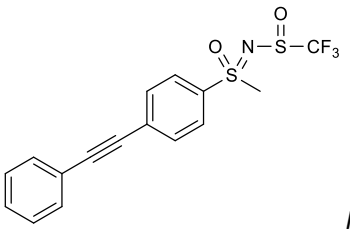
S-(4'-methyl-[1,1'-biphenyl]-4-yl)-*S*-methyl sulfoximine (**1af**). **3g** (0.1 mmol; 35 mg), 1.33 equiv. 4-methylphenyl boronic acid (0.133 mmol, 18 mg), 3 equiv. K_2CO_3 (0.3 mmol, 41 mg), catalytic amount of Pd/C: White solid (22 mg, 90%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.09 – 7.99 (m, 2H), 7.76 – 7.71 (m, 2H), 7.54 – 7.46 (m, 2H), 7.33 – 7.28 (m, 2H), 3.15 (s, 3H), 2.41 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 146.18, 141.67, 138.76, 136.43, 129.93, 128.36, 127.77, 127.31, 46.38, 21.30. **IR (neat)**: ν 3297, 3204, 3064, 3004, 2921, 1590, 1558, 1524, 1484, 1409, 1393, 1323, 1310, 1220, 1133, 1112, 1090, 996, 967, 940, 845, 807, 752, 727, 712 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{16}NOS$ 246.0947; Found 246.0943. Mp = 161.9 – 163.4 °C. The compound contains 5% **1g**, which we were unable to separate from the product.



N-(trifluoromethylsulfaneylidene)-*S*-(4'-methyl-[1,1'-biphenyl]-4-yl)-*S*-methyl sulfoximine (**3af**). **3g** (0.2 mmol; 70 mg), 1.1 equiv 4-methylphenyl boronic acid (0.22 mmol, 30 mg), 5 equiv. K_2CO_3 (1.0 mmol, 136 mg), 10 mol% XPhos (0.02 mmol, 10 mg), 10 mol% $Pd(OAc)_2$ (0.02 mmol, 5 mg). **IR (neat)**: ν 3009, 2923, 1594, 1519, 1484, 1391, 1315, 1231, 1170, 1153, 1093, 1043, 1001, 971, 852, 826, 809, 780, 746, 705, 615 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{15}F_3NO_2S_2$ 362.0491; Found 362.0487.

Diastereoisomer 1 (**3af-1**): white solid (30 mg, 42%) **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.08 – 7.98 (m, 2H), 7.87 – 7.78 (m, 2H), 7.55 – 7.50 (m, 2H), 7.34 – 7.29 (m, 2H), 3.46 (s, 3H), 2.43 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-d) δ −80.49. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 148.03, 139.46, 136.21, 135.70, 130.09, 128.30, 128.11, 127.39, 124.12 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz), 47.58, 21.34. Mp = 133.9 – 135.1 °C.

Diastereoisomer 2 (**3af-2**): white solid (24mg, 33%) **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.11 – 8.05 (m, 2H), 7.85 – 7.79 (m, 2H), 7.55 – 7.47 (m, 2H), 7.37 – 7.29 (m, 2H), 3.41 (s, 3H), 2.43 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-d) δ −80.85. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 148.25, 139.46, 135.73, 135.59, 130.10, 128.92, 128.47, 127.42, 124.07 (C-F, $^1J_{C\text{-}F}$ = 333.7 Hz), 47.30, 21.35. Mp = 156.0 – 156.9 °C.

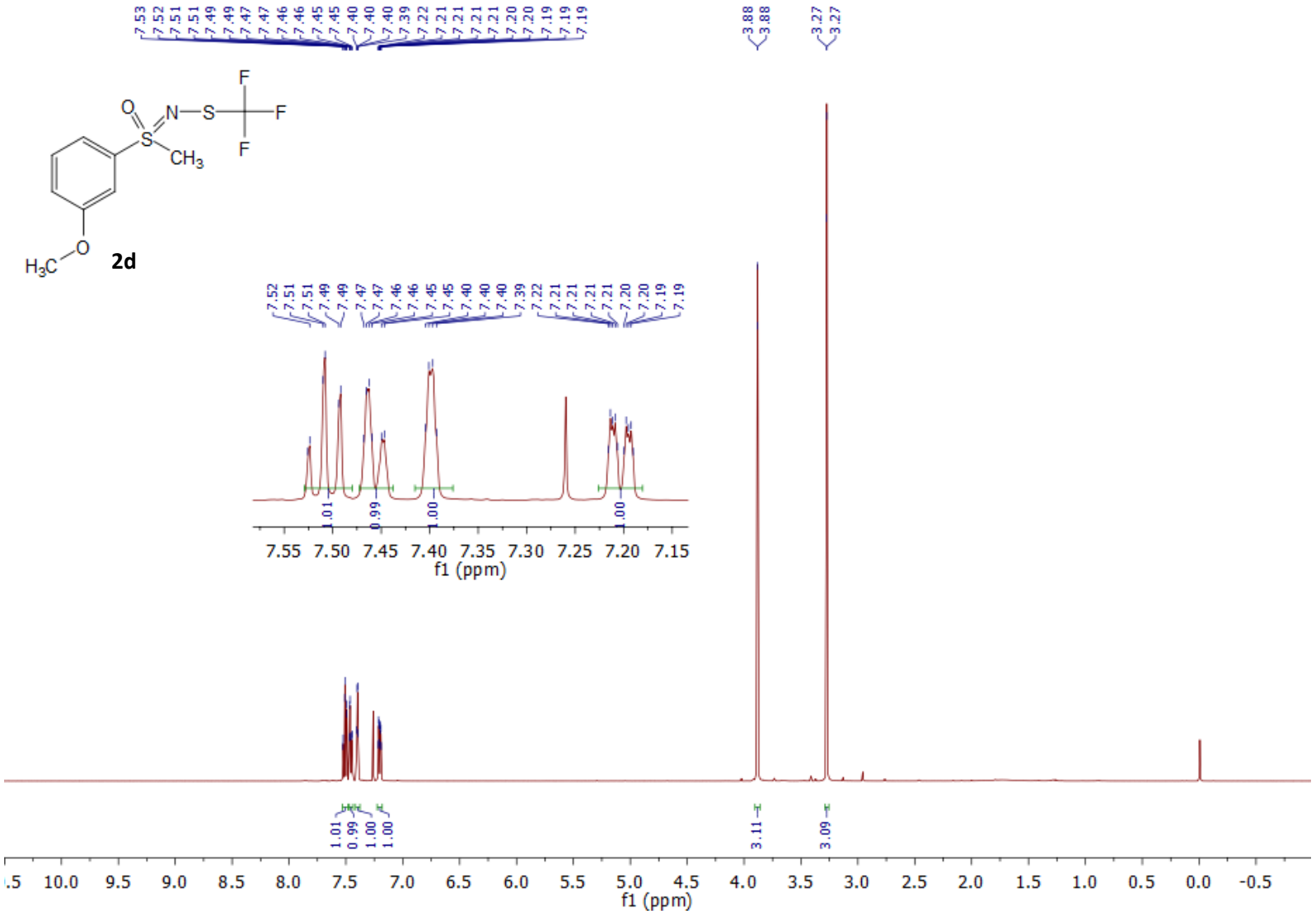


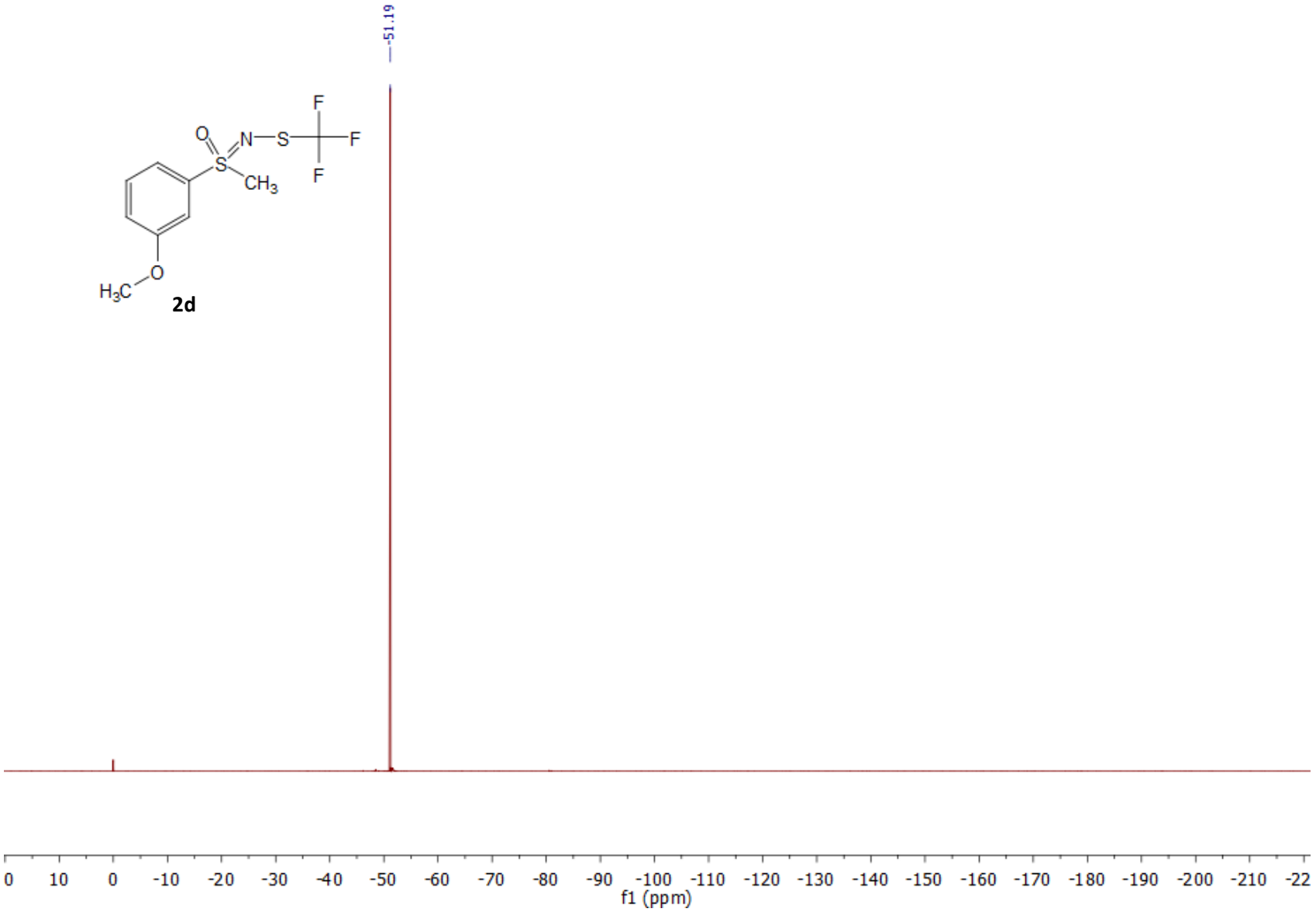
N-(trifluoromethylsulfaneylidene)-*S*-(4-(phenylethynyl)phenyl)-*S*-methyl sulfoximine (**3ag**). **3g** (0.3 mmol; 105 mg), 1.3 equiv phenylacetylene (0.39 mmol, 40 mg), 10 mol% $PdCl_2(PPh_3)_2$ (0.03 mmol, 21 mg), 10 mol% CuI (0.03 mmol, 6 mg). **IR (neat)**: ν 3084, 3059, 3010, 2990, 2926, 2910, 2216, 1586, 1497, 1444, 1399, 1328, 1225, 1183, 1149, 1086, 1023, 998, 923, 838, 786, 755, 710, 689, 610 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{16}H_{13}F_3NO_2S_2$ 372.0334; Found 372.0331.

Diastereoisomer 1 (**3ag-1**): orange solid (43 mg, 39%) **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 8.06 – 8.01 (m, 2H), 7.79 – 7.74 (m, 2H), 7.59 – 7.53 (m, 2H), 7.44 – 7.36 (m, 3H), 3.39 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-d) *δ* −80.80. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 136.62, 132.94, 132.05, 130.91, 129.52, 128.68, 128.35, 124.03 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz), 122.04, 94.93, 87.33, 47.16. Mp = 130.0 – 130.3 °C.

Diastereoisomer 2 (**3ag-2**): orange semi solid (33 mg, 30%) **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 7.99 – 7.94 (m, 2H), 7.79 – 7.73 (m, 2H), 7.59 – 7.54 (m, 2H), 7.44 – 7.32 (m, 3H), 3.44 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-d) *δ* −80.47. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 137.11, 132.83, 132.02, 130.69, 129.54, 128.69, 127.58, 124.07 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz), 122.01, 94.86, 87.28, 47.41.

Copies of ^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra of products

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F
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-30
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-50
-60
-70
-80
-90
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-110
-120
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-140
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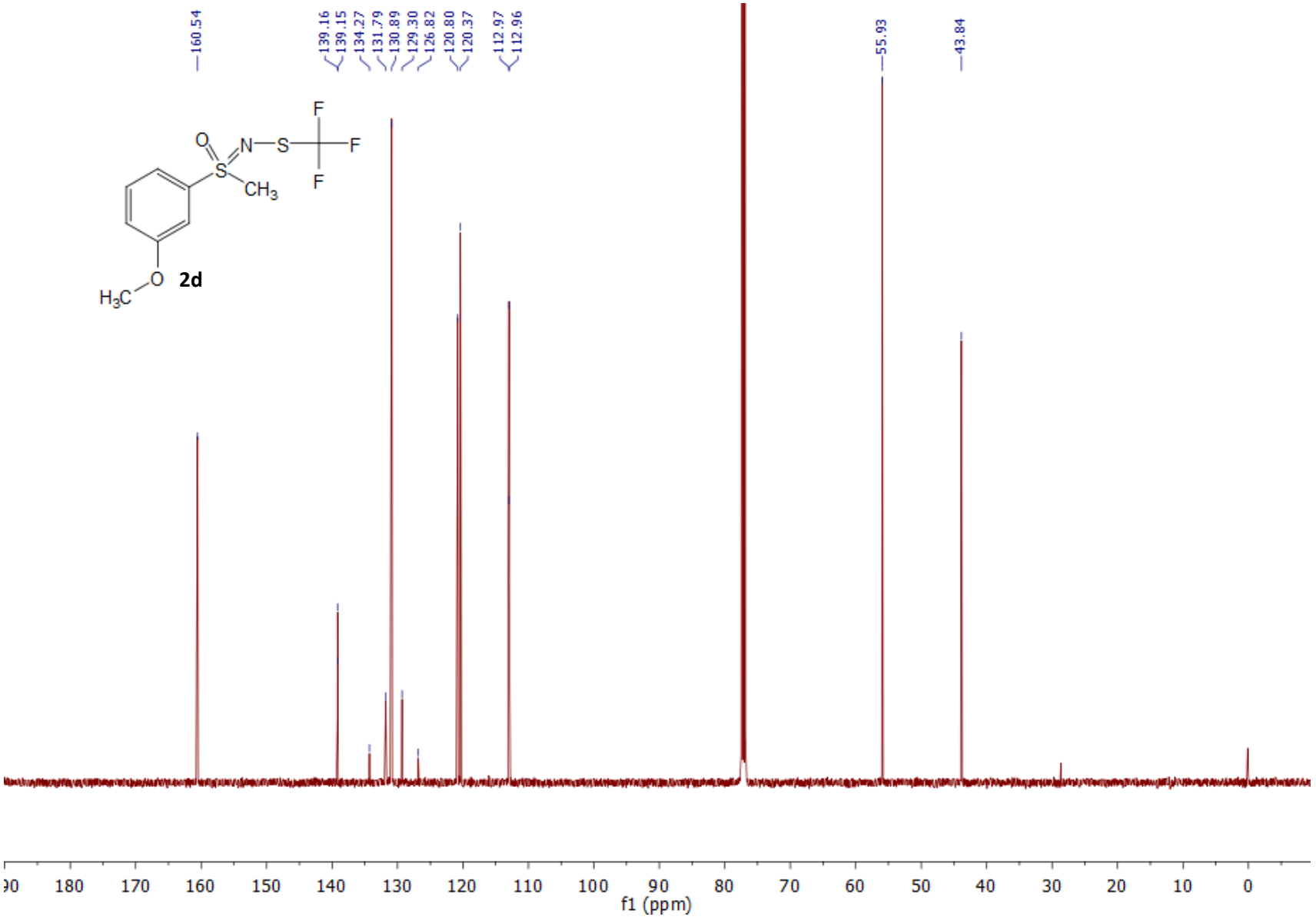
-200
-210
-22
f1 (ppm)

2d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55.93
43.84
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O
N
S
F
S
CH3
F
H3C
O
2d
90
180
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110
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90
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70
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50
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30
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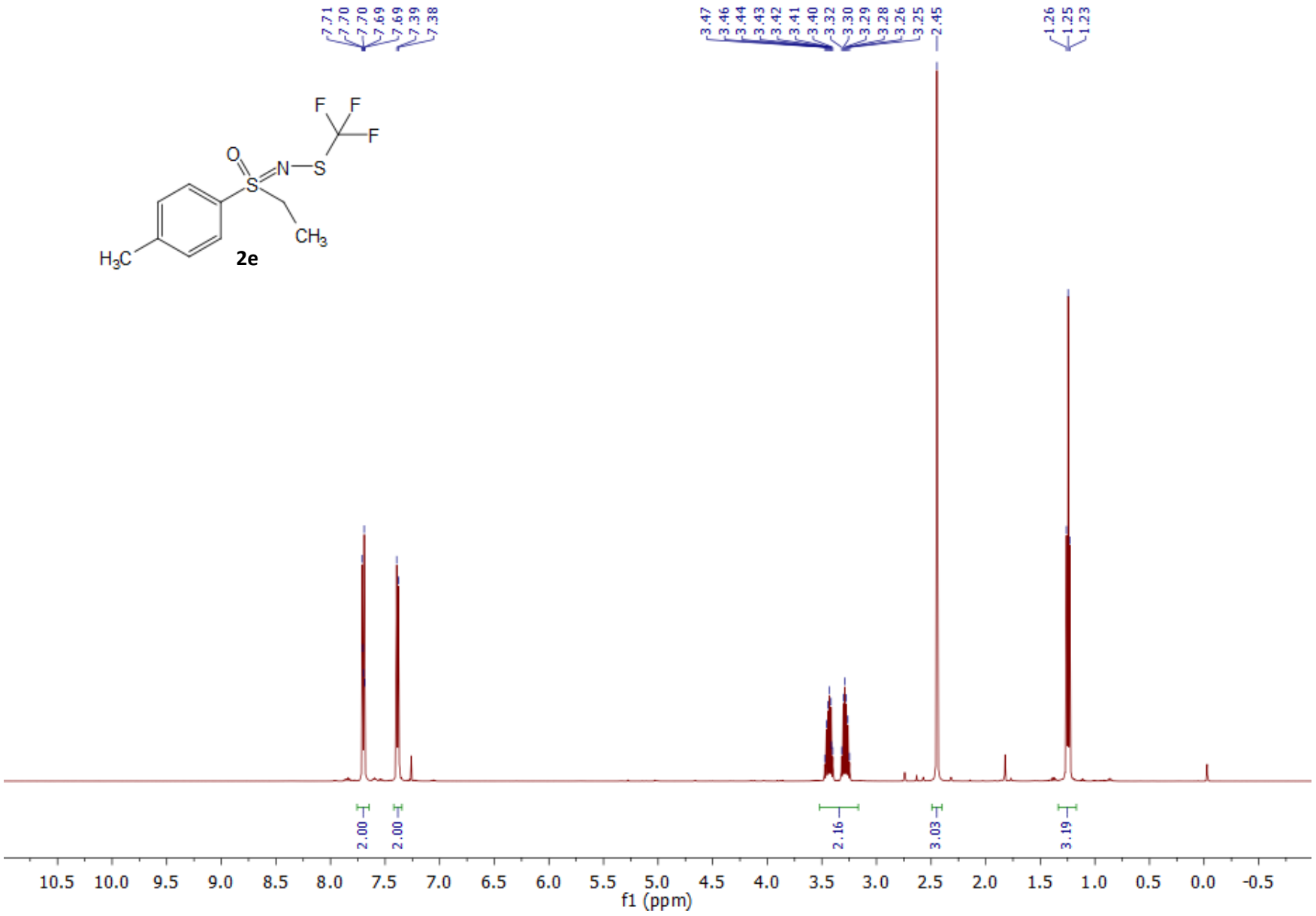
10
0
f1 (ppm)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3.40
3.32
3.30
3.29
3.28
3.26
3.25
2.45
1.26
1.25
1.23
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F
F
O
N
S
S
CH3
H3C
2e
2.00
2.00
2.16
3.03
3.19
10.5
10.0
9.5
9.0
8.5
8.0
7.5
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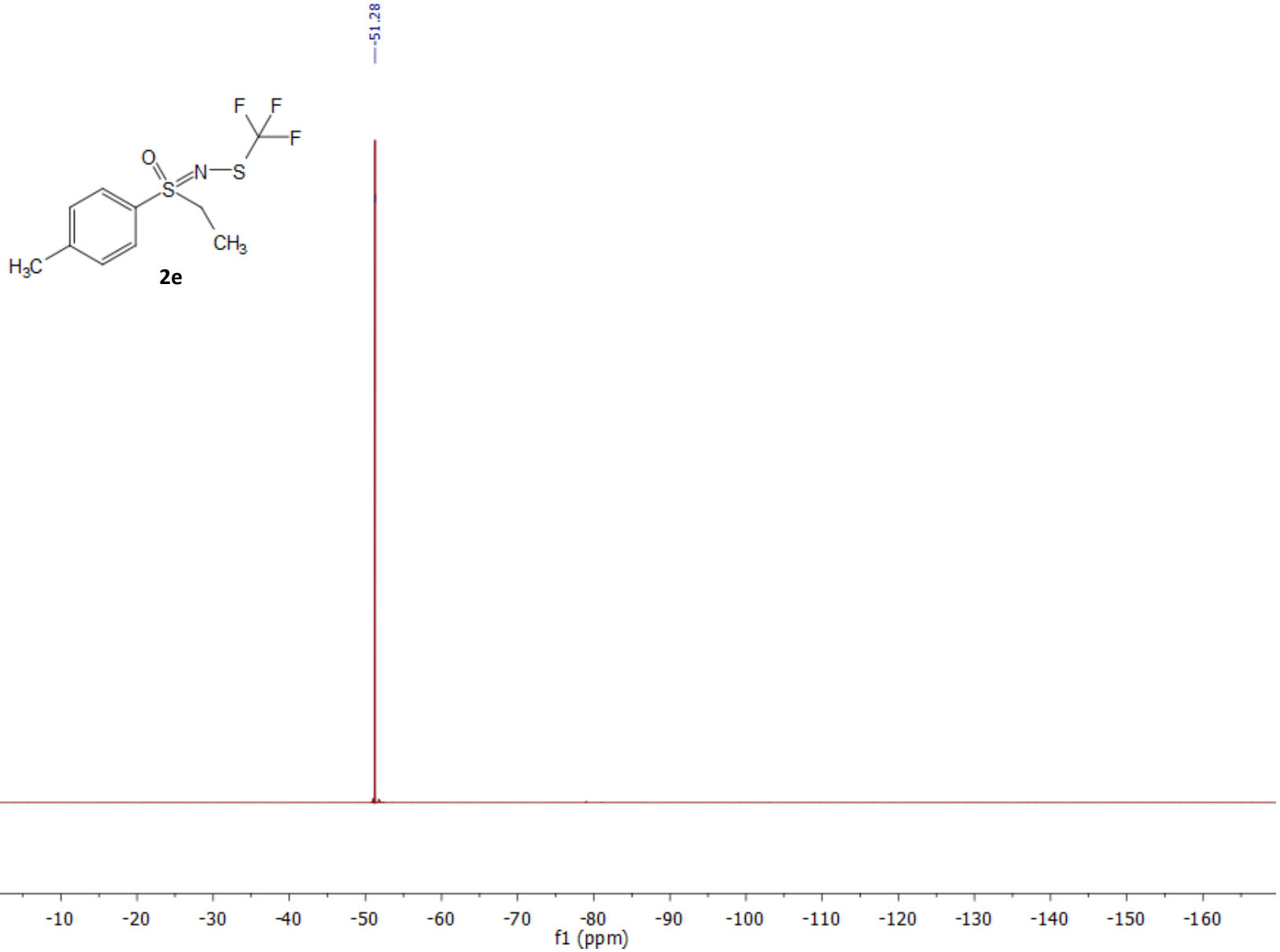
f1 (ppm)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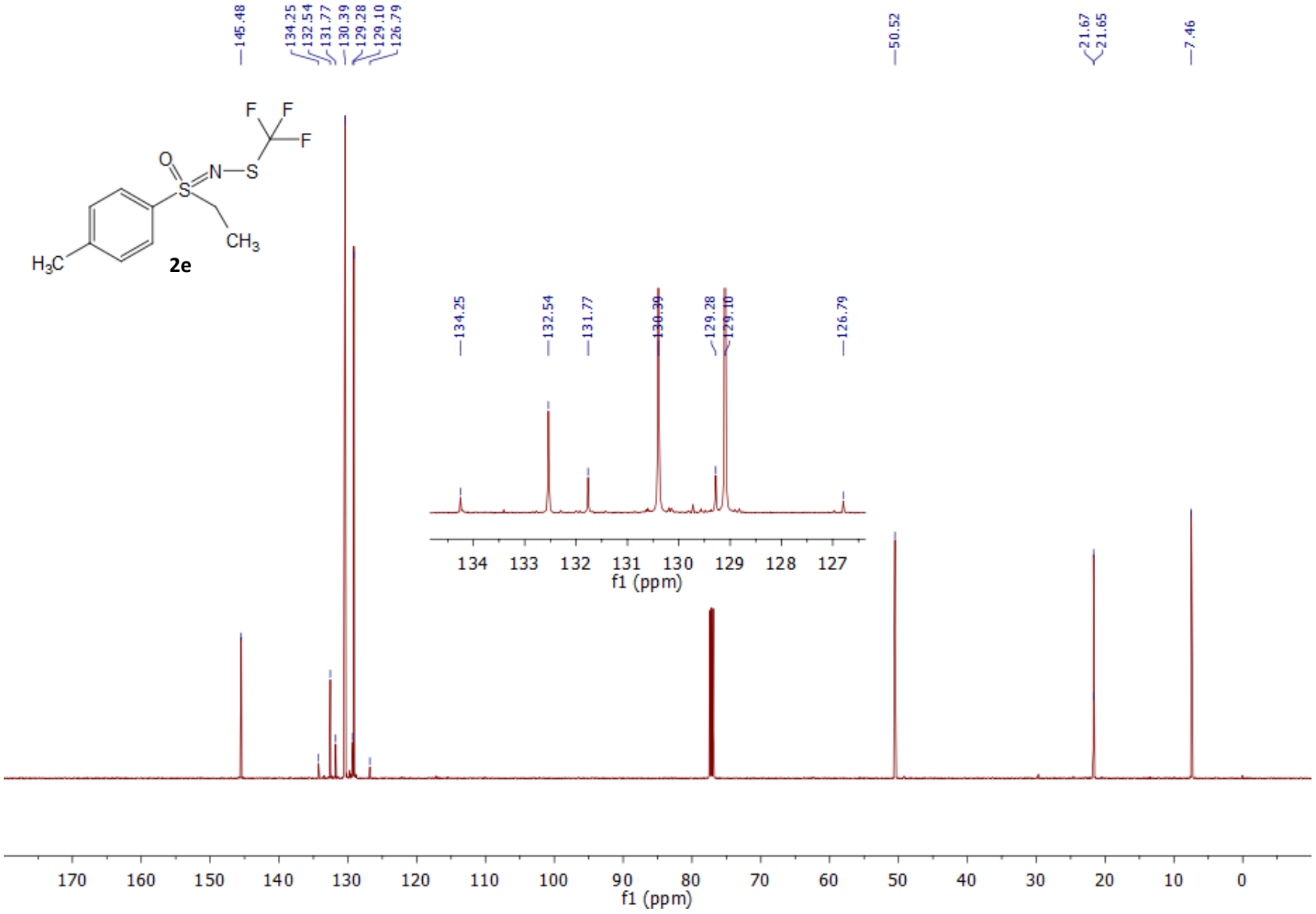
f1 (ppm)

2e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F
F
O
N
S
S
CH3
H3C
2e
134.25
132.54
131.77
130.39
129.28
129.10
126.79
134 133 132 131 130 129 128 127
f1 (ppm)
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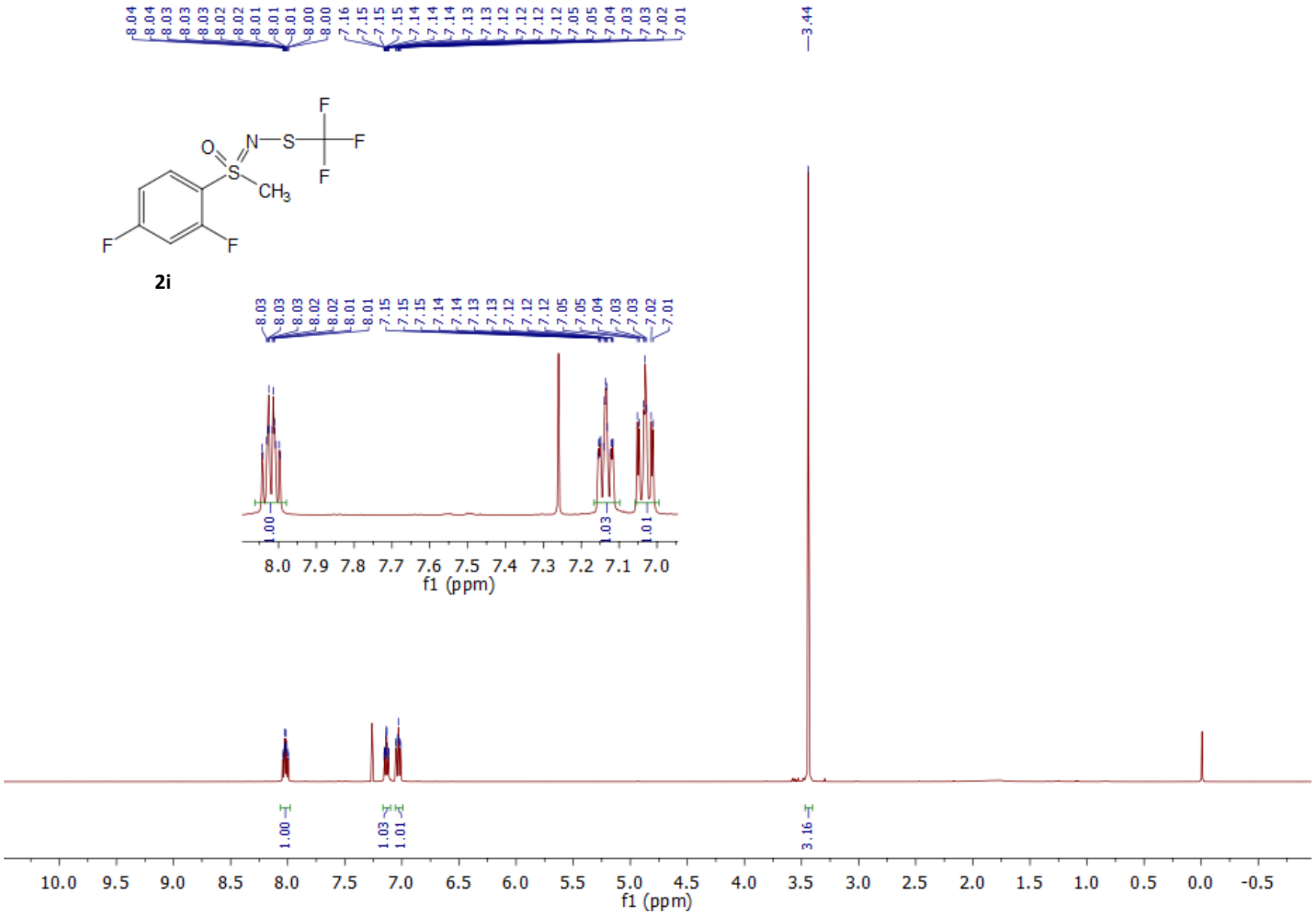
f1 (ppm)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3.44
F
O
N
S
F
F
S
CH3
F
F
2i
8.03 8.03 8.03 8.02 8.02 8.01 8.01
7.15 7.15 7.15 7.14 7.14 7.13 7.13 7.12 7.12 7.12 7.05 7.05 7.04 7.03 7.03 7.02 7.01
1.00
1.03
1.01
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
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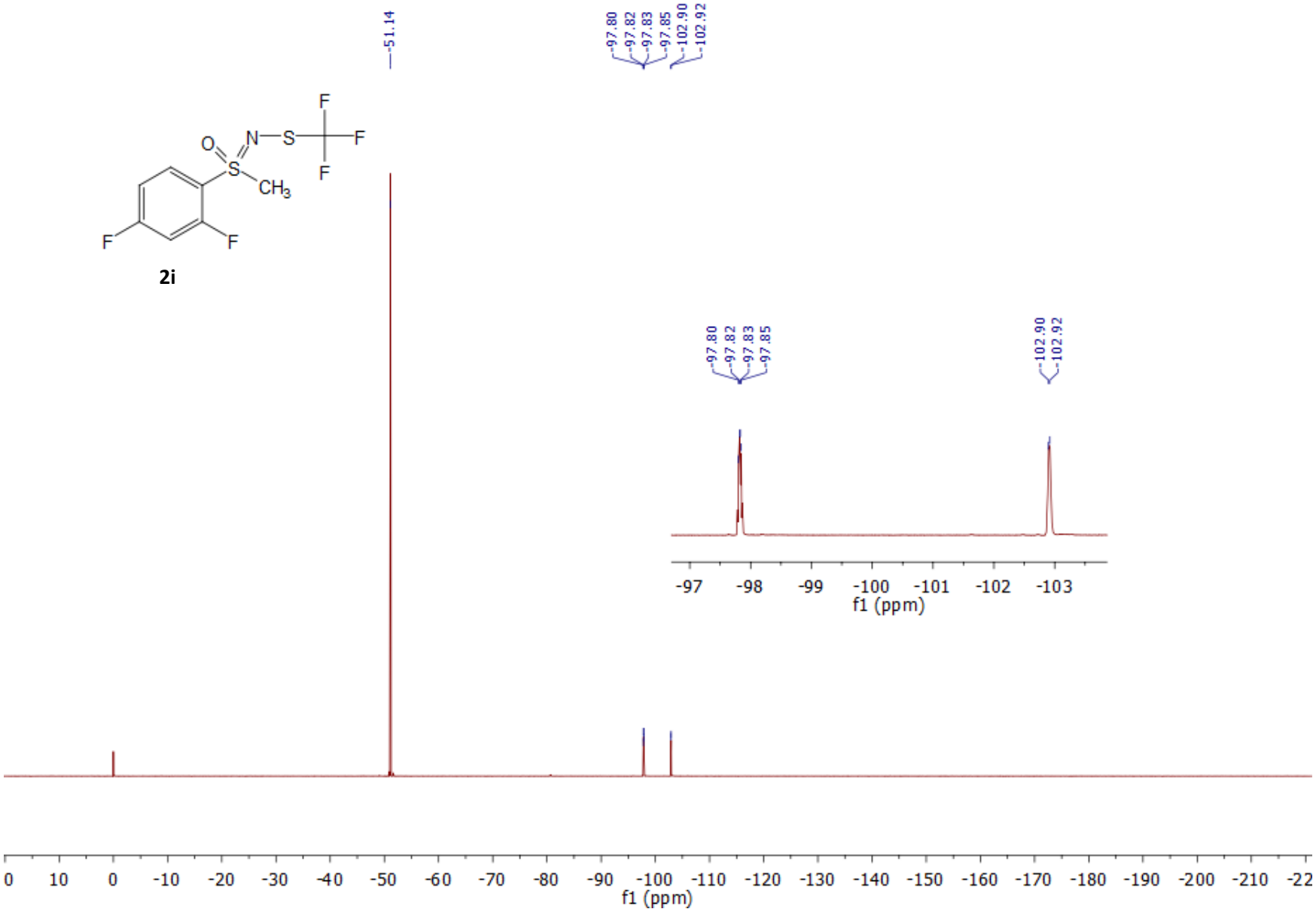
1.03
1.01
3.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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-97.85
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-102.92
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O
N
S
F
F
S
CH3
F
F
2i
-97.80
-97.82
-97.83
-97.85
-102.90
-102.92
-97 -98 -99 -100 -101 -102 -103
f1 (ppm)
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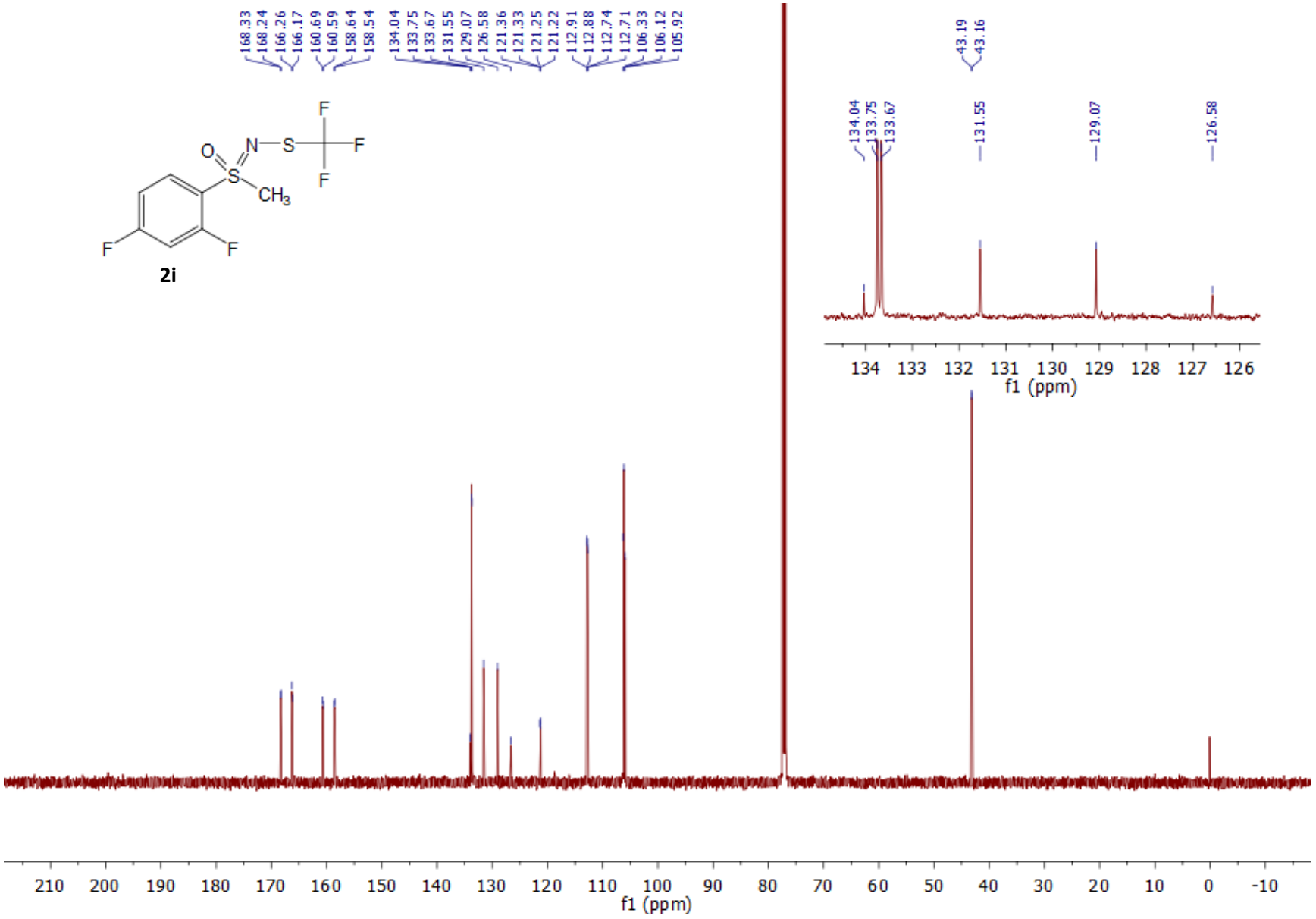
f1 (ppm)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106.33
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43.16
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N
S
F
F
F
S
CH3
F
F
2i
134.04
133.75
133.67
131.55
129.07
126.58
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f1 (ppm)
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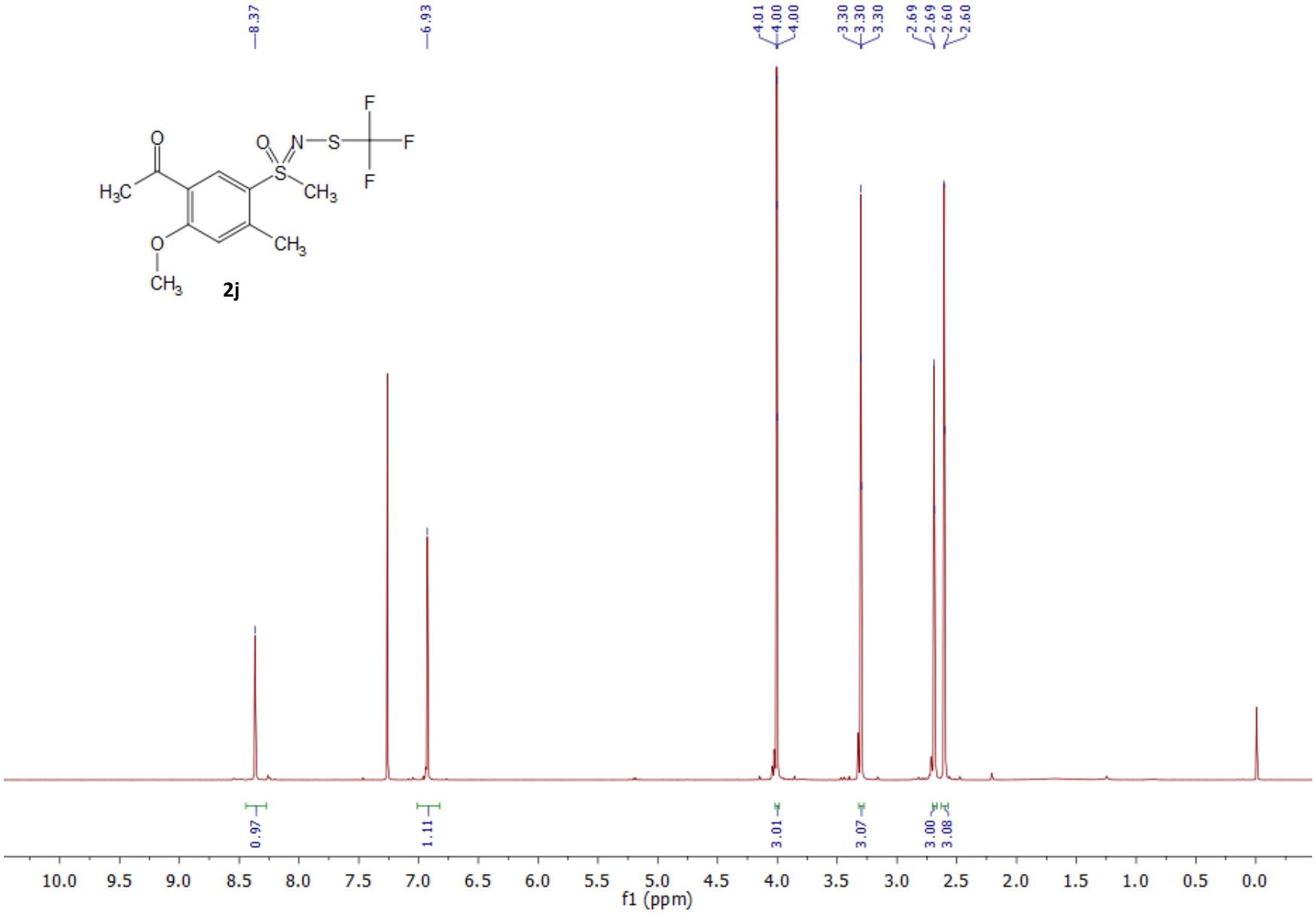
f1 (ppm)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H3C
O
N
S
F
F
F
S
CH3
O
CH3
CH3
2j
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1.11
3.01
3.07
3.00
3.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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6.0
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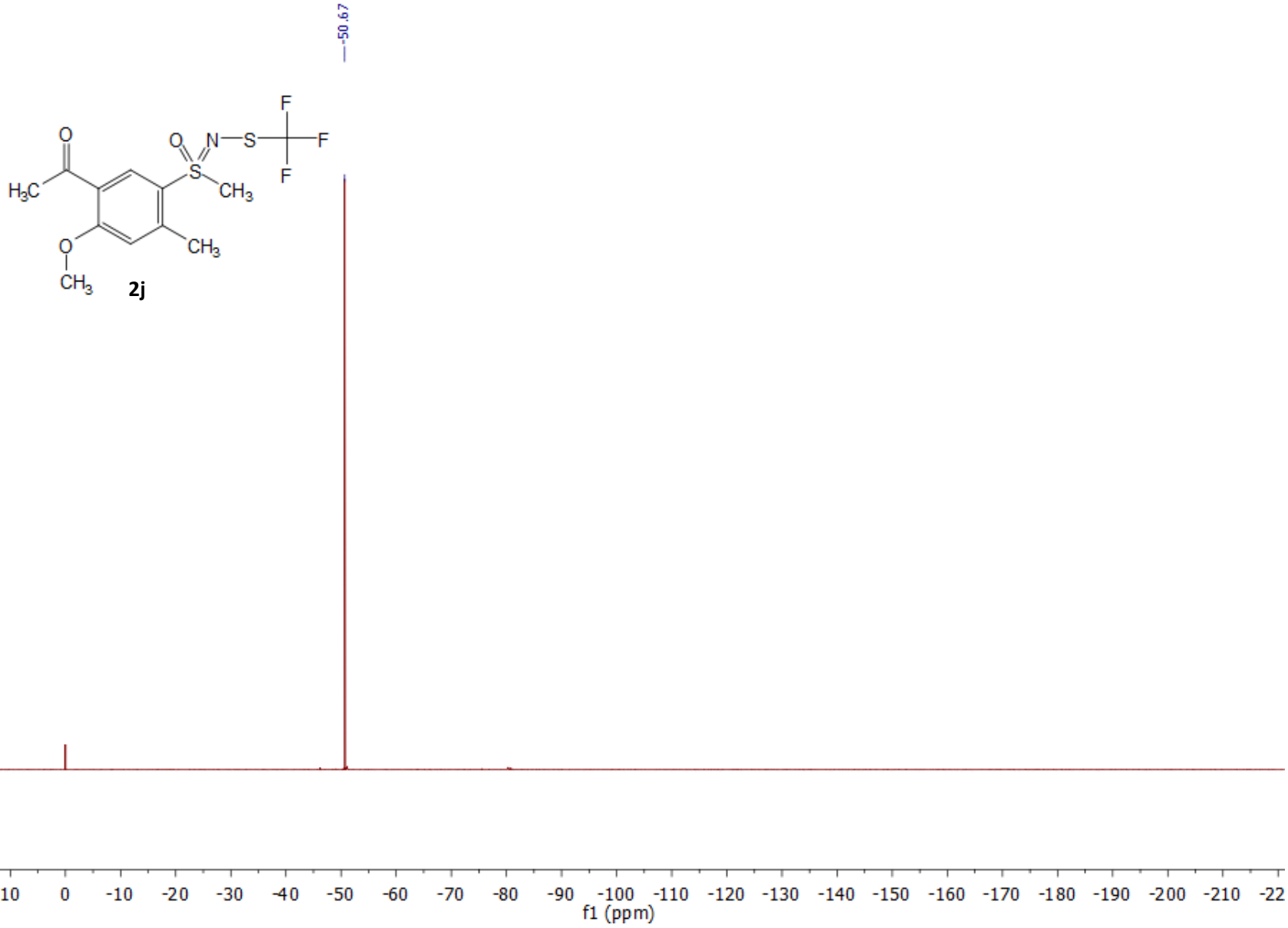
f1 (ppm)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-80
-90
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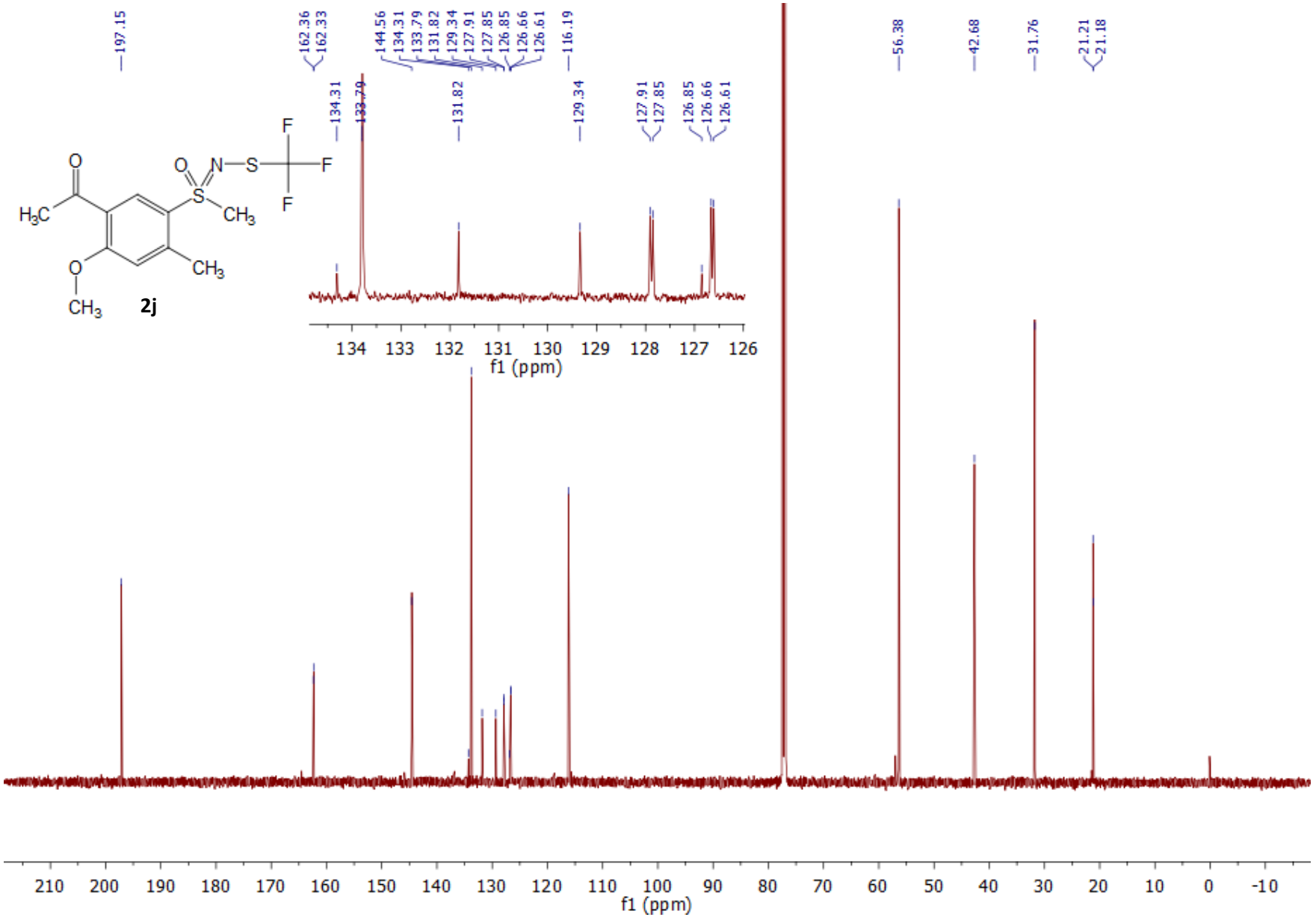
f1 (ppm)

2j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133
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128
127
126
f1 (ppm)
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190
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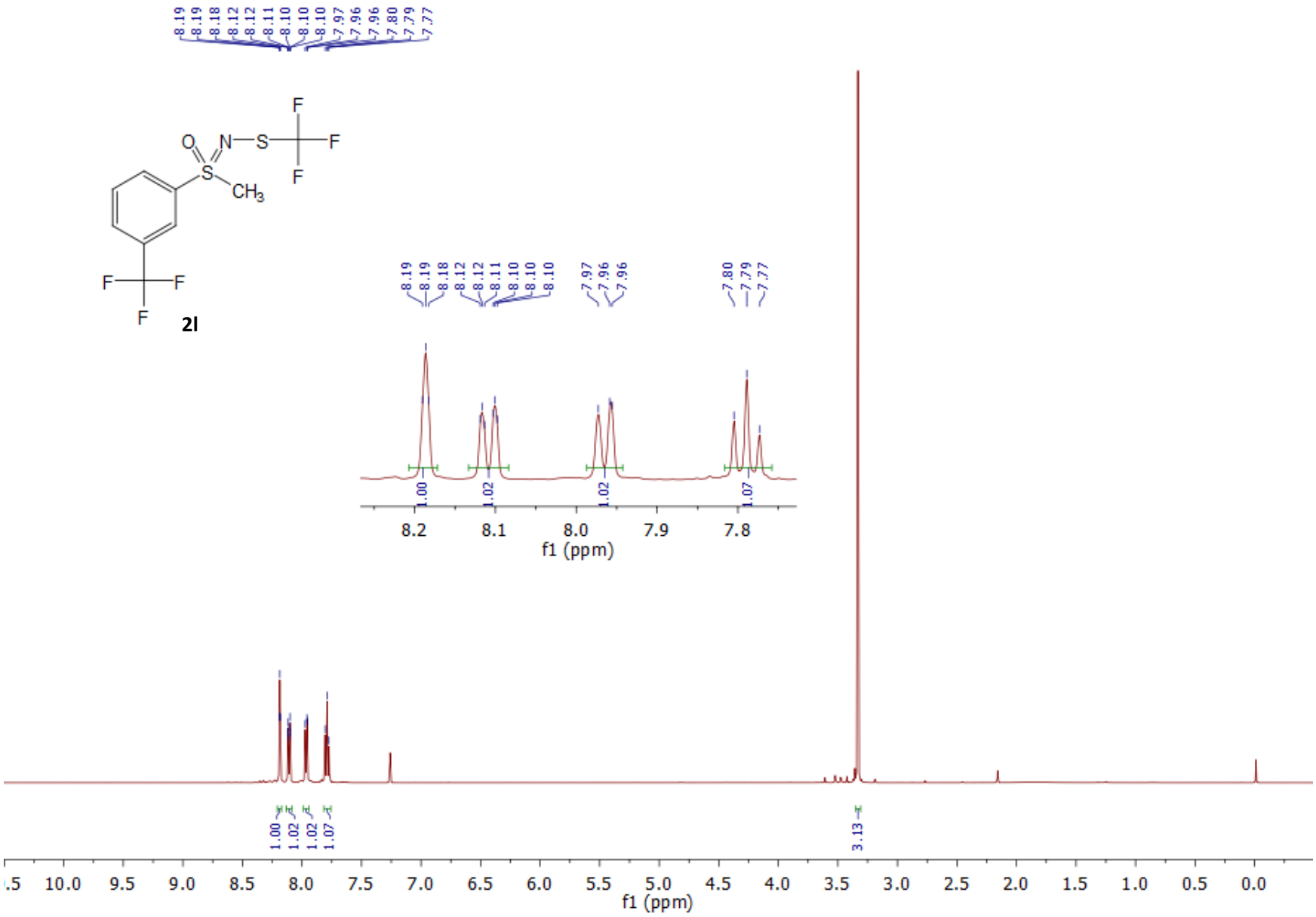
f1 (ppm)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O
N
S
S
CH3
F
F
F
2l
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1.02
1.07
8.2
8.1
8.0
7.9
7.8
f1 (ppm)
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
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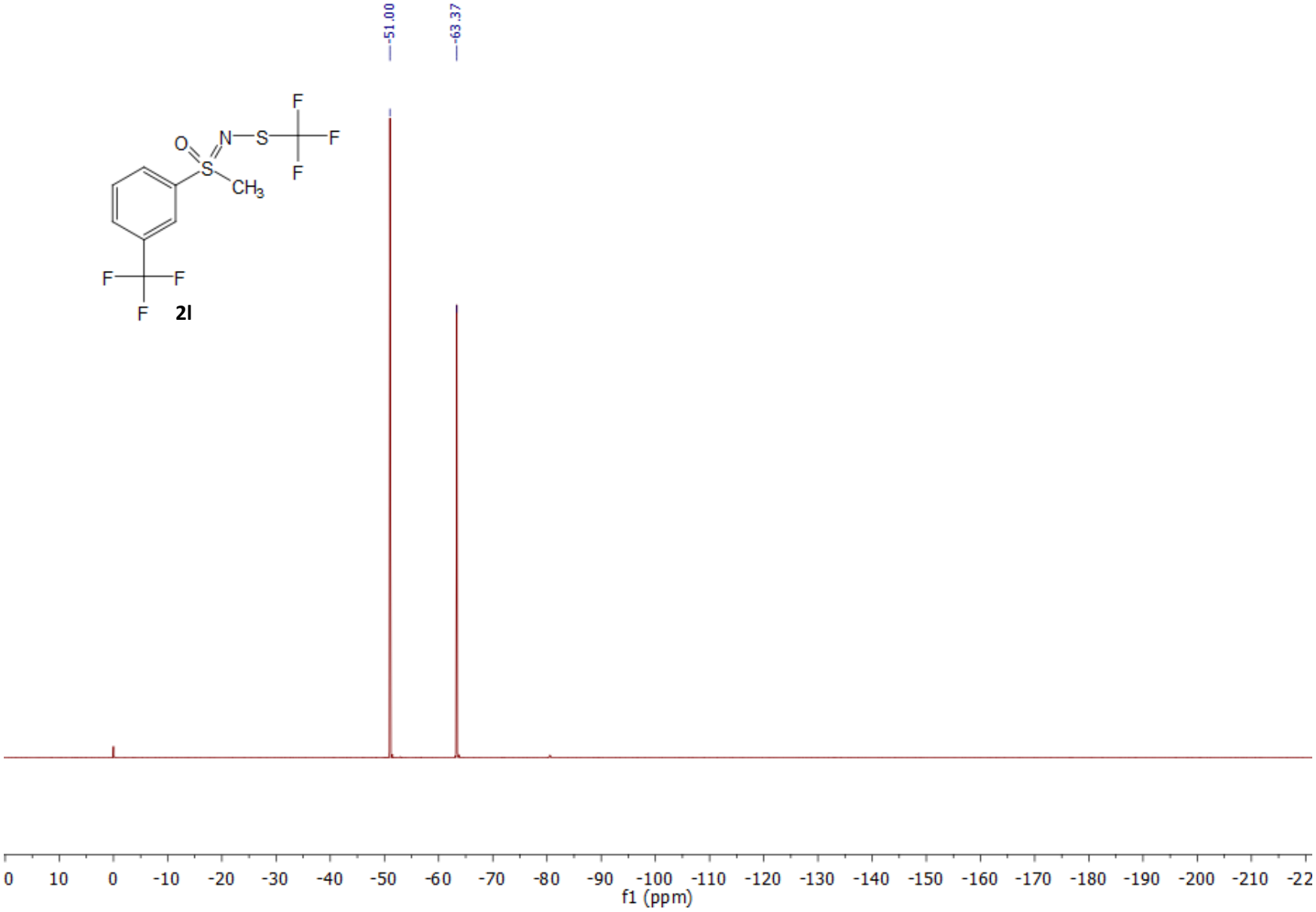
0.0
f1 (ppm)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S
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F
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2l
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-70
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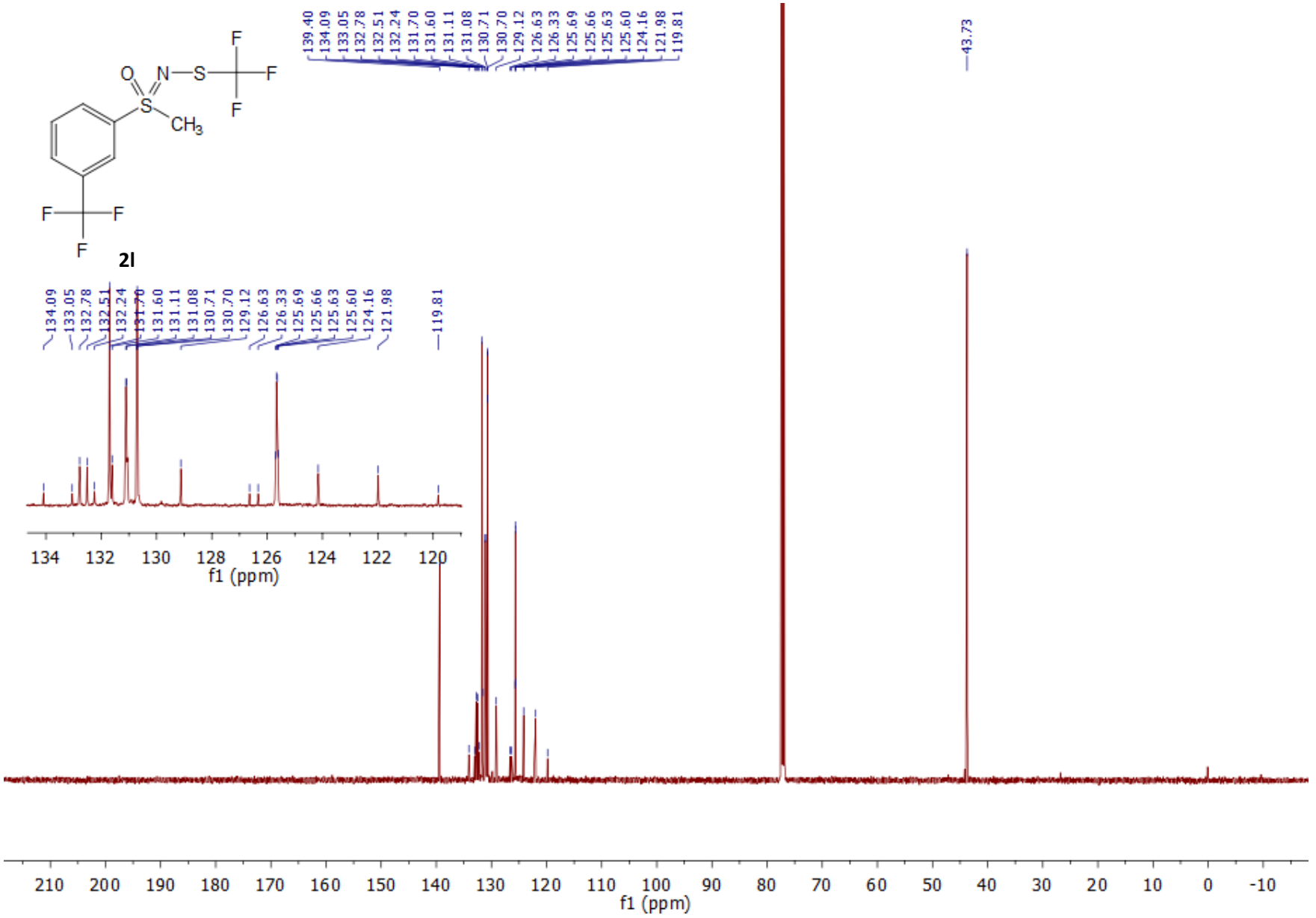
-22
f1 (ppm)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129.12
126.63
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125.63
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119.81
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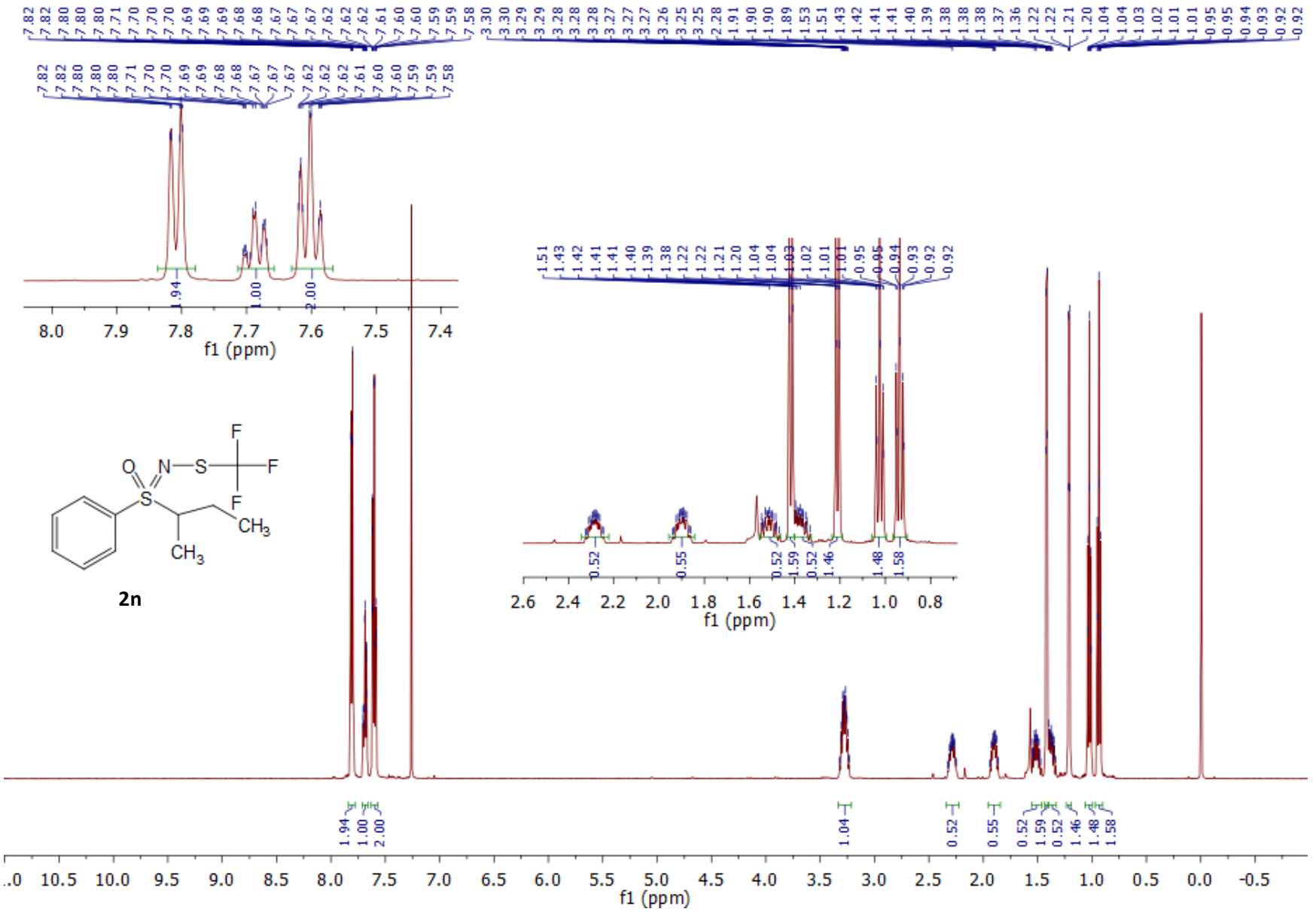
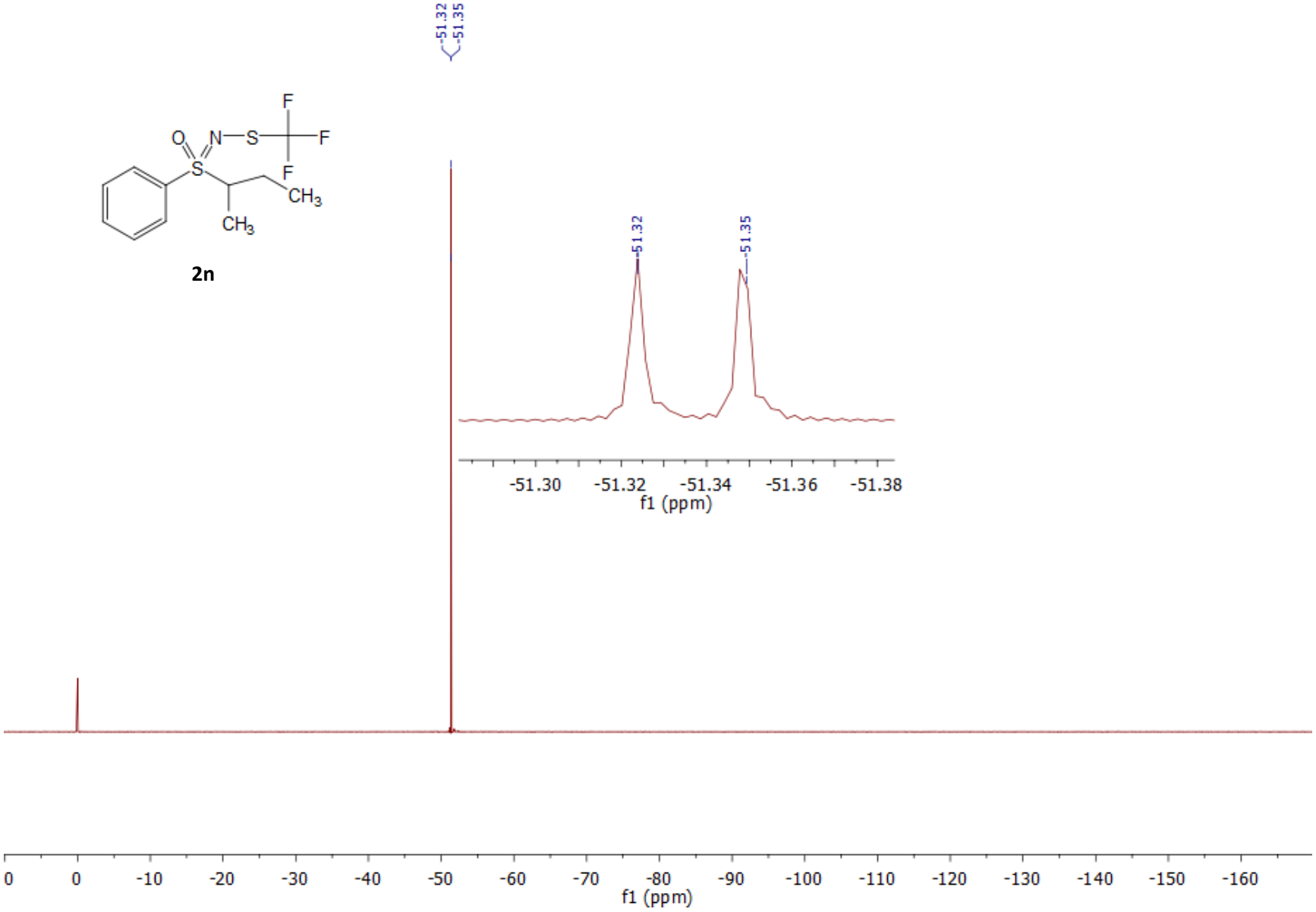
f1 (ppm)
f1 (ppm)



2n

F
O
N
S
F
S
F
CH3
CH3

2n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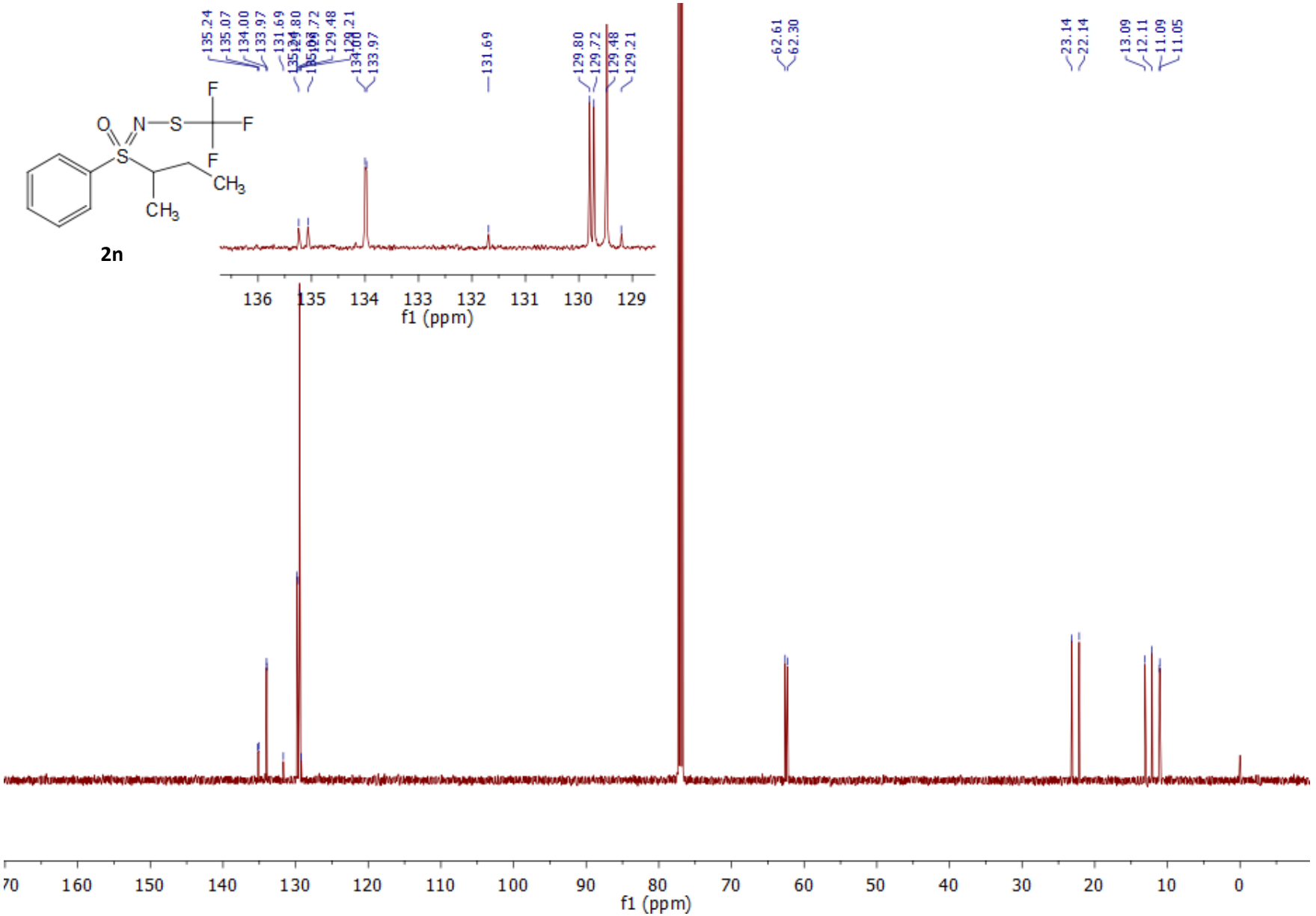
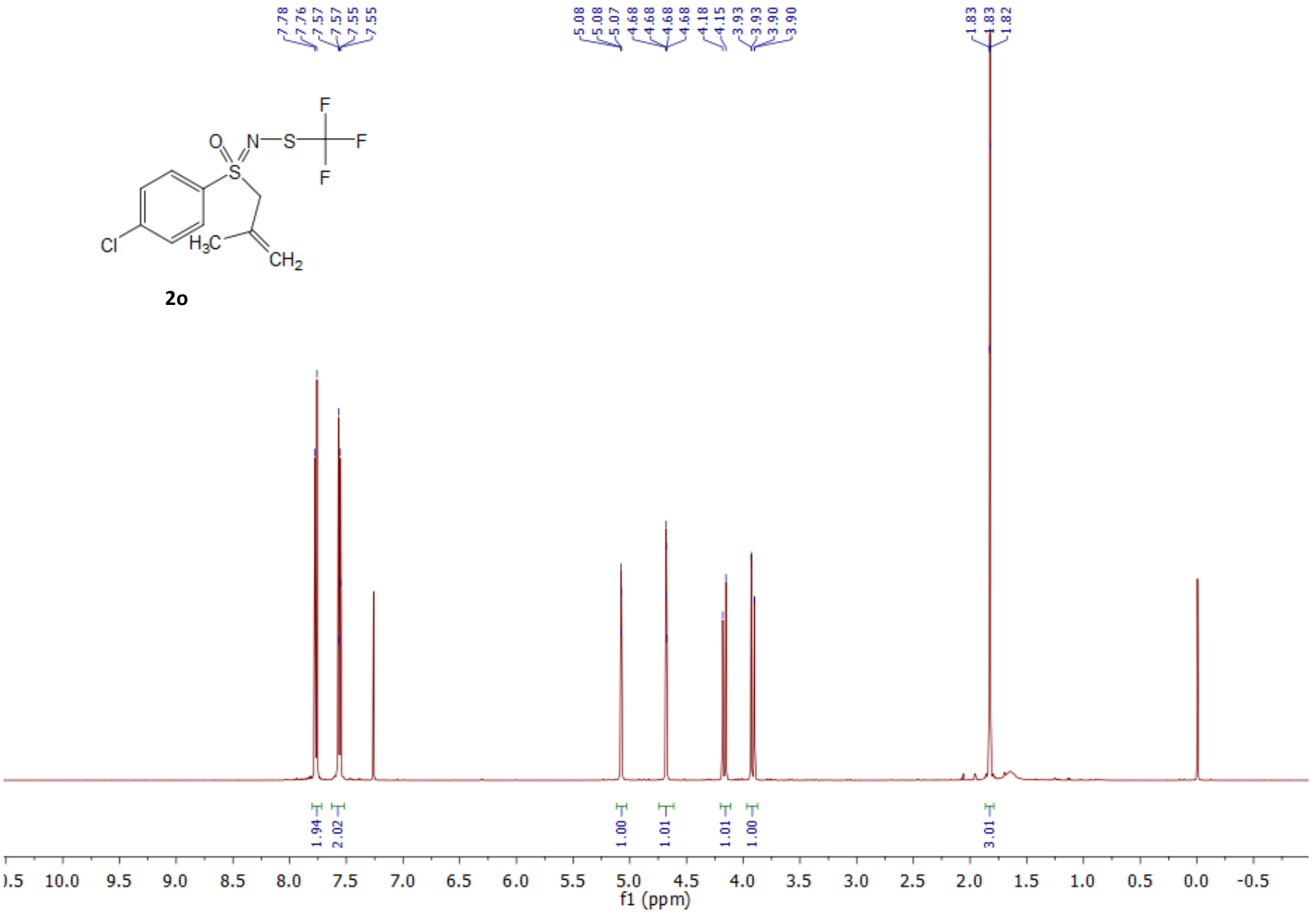
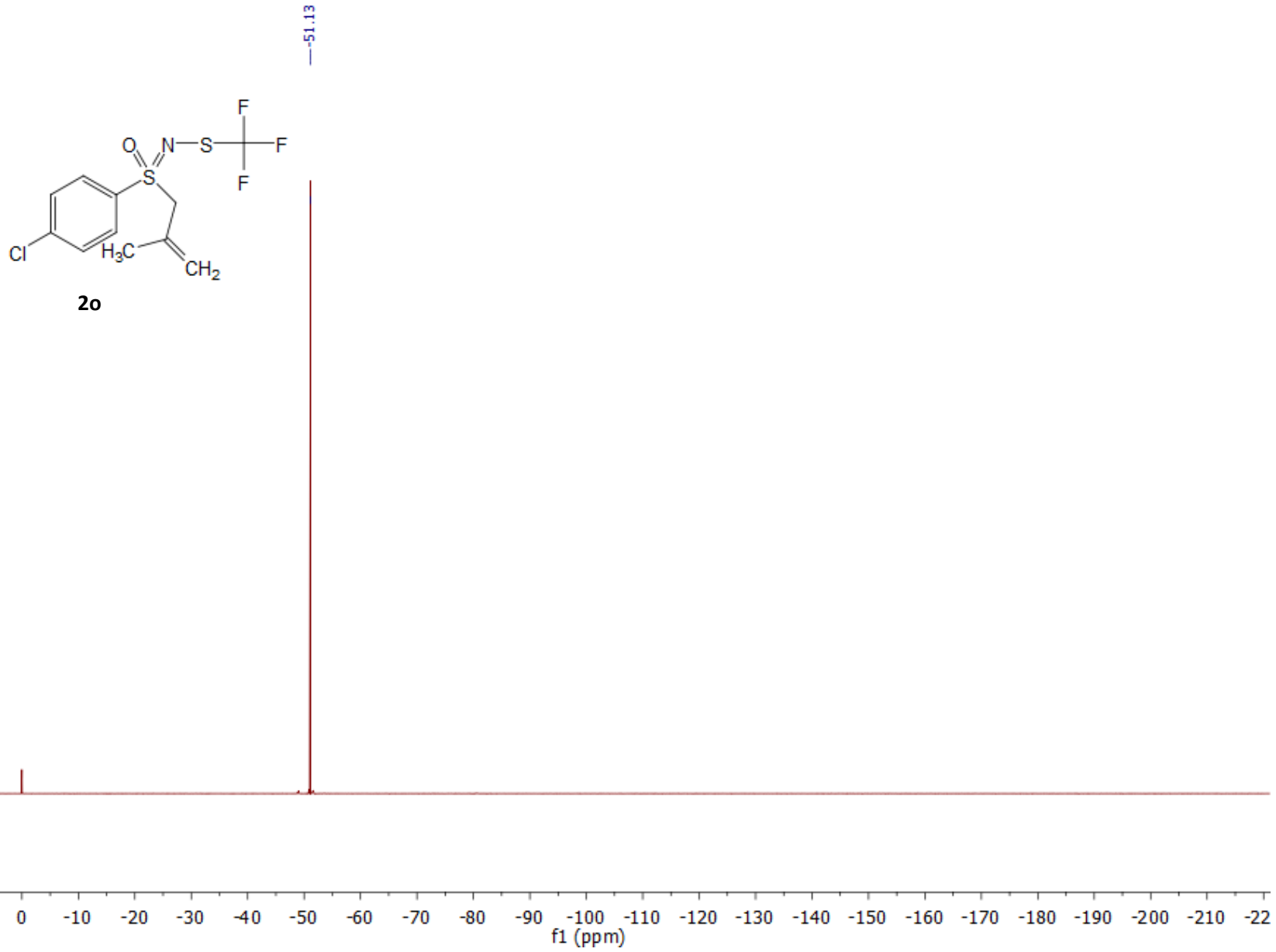
-90
-100
-110
-120
-130
-140
-150
-160
f1 (ppm)


135.24
135.07
134.00
133.97
131.69
129.80
129.72
129.48
129.21
62.61
62.30
23.14
22.14
13.09
12.11
11.09
11.05
O
N
S
F
F
F
S
CH3
CH3
2n
136
135
134
133
132
131
130
129
f1 (ppm)
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.78
7.76
7.57
7.57
7.55
7.55
5.08
5.08
5.07
4.68
4.68
4.68
4.68
4.18
4.15
3.93
3.93
3.90
3.90
1.83
1.83
1.82
F
F
F
O
N
S
S
Cl
H3C
CH2
1.94
2.02
1.00
1.01
1.01
1.00
3.01
f1 (ppm)

2o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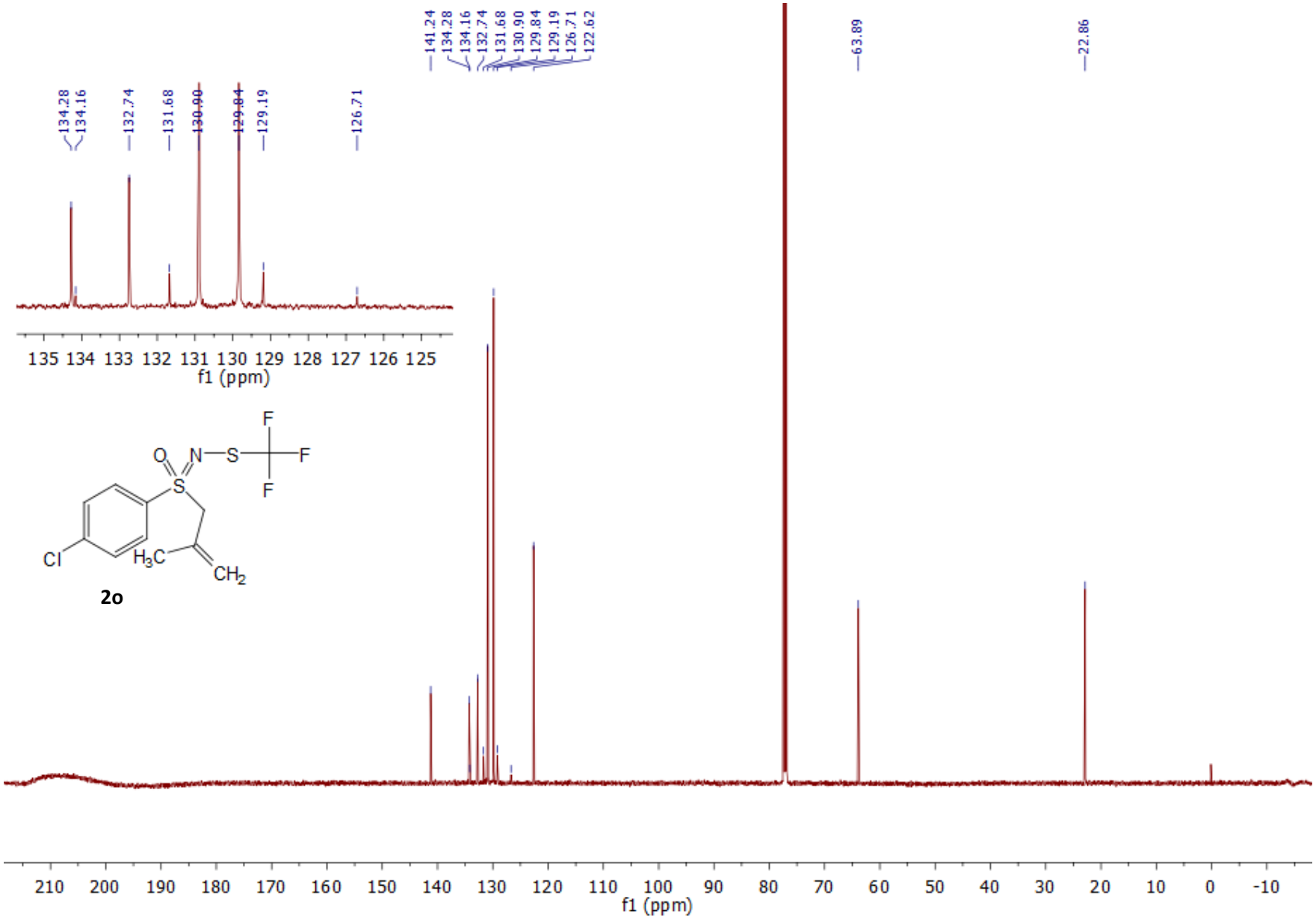
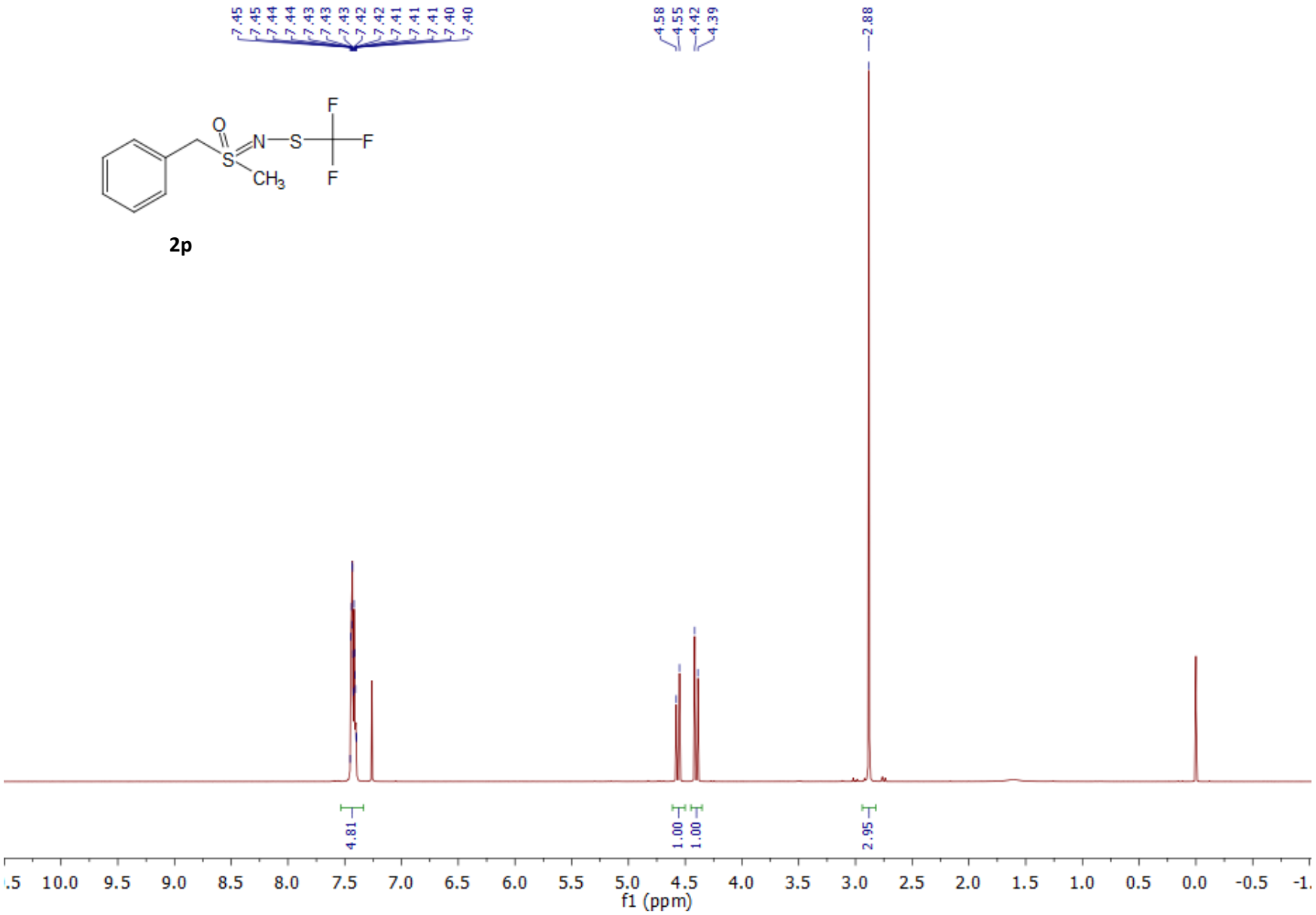
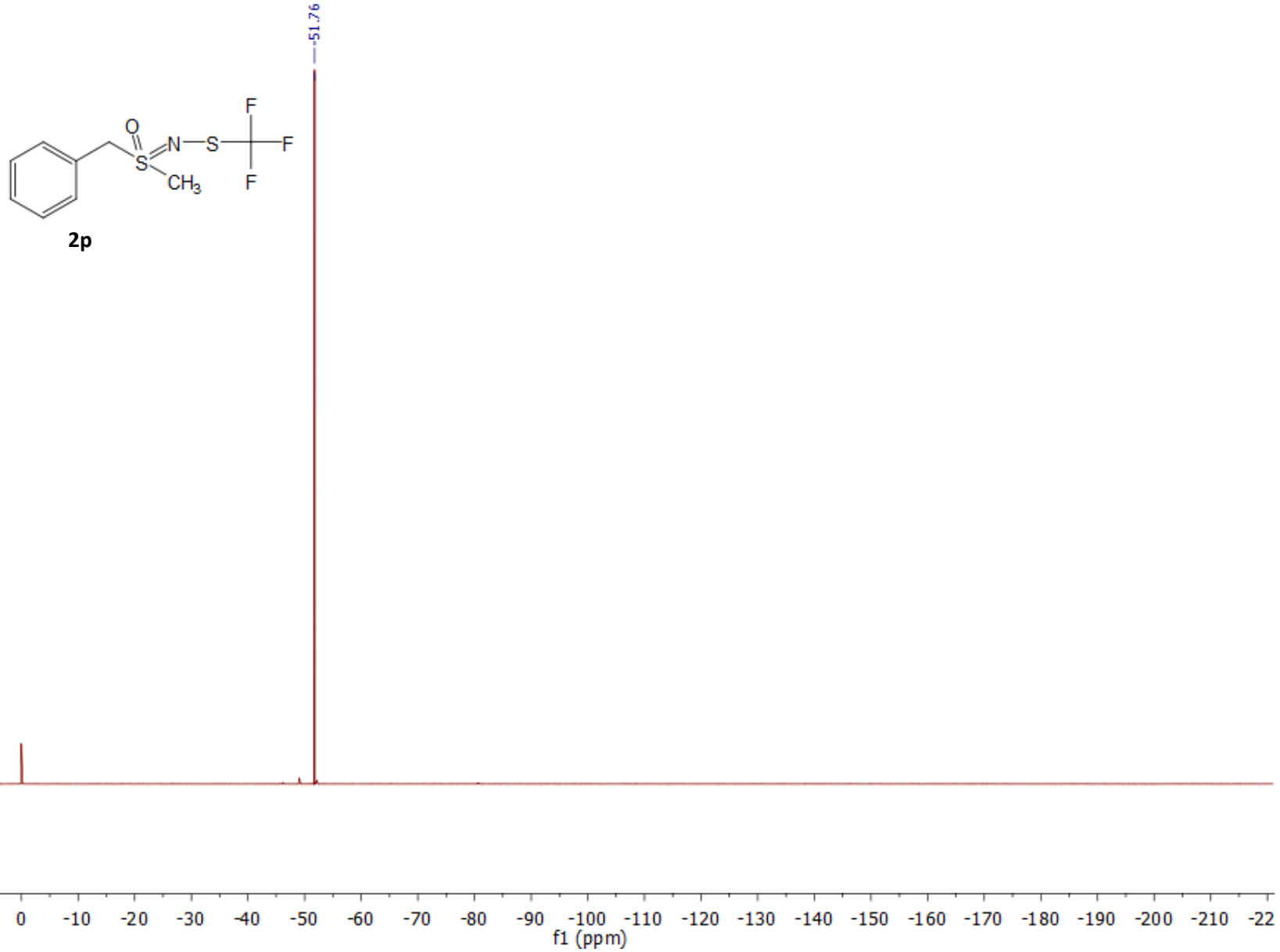
F
O
N
S
F
S
F
Cl
H3C
CH2
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

2o

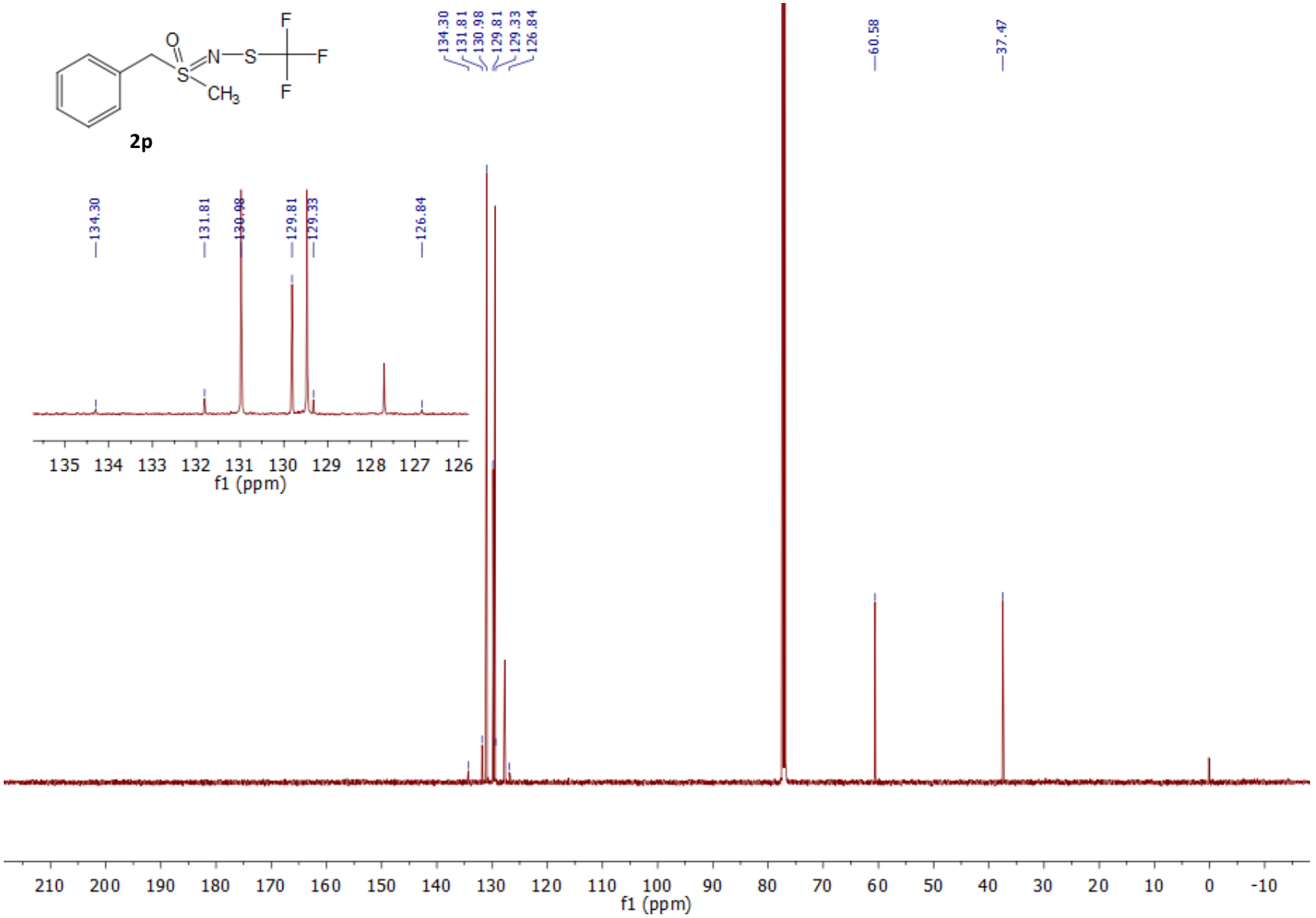

141.24
134.28
134.16
132.74
131.68
130.90
129.84
129.19
126.71
122.62
63.89
22.86
134.28
134.16
132.74
131.68
130.90
129.84
129.19
126.71
135 134 133 132 131 130 129 128 127 126 125
f1 (ppm)
F
O
N
S
F
S
F
Cl
H3C
CH2
2o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

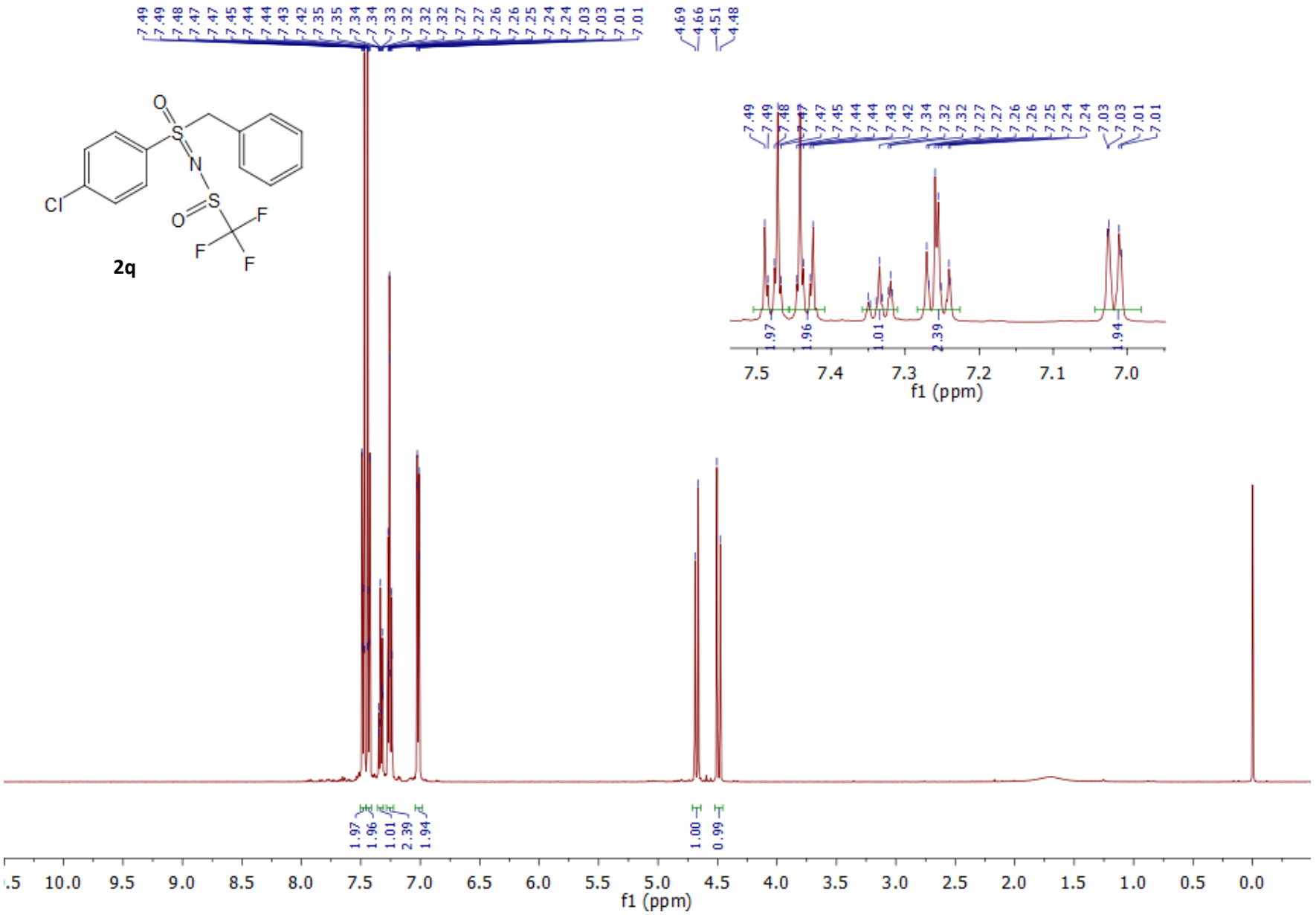

7.45
7.45
7.44
7.44
7.43
7.43
7.43
7.42
7.42
7.41
7.41
7.41
7.40
7.40
4.58
4.55
4.42
4.39
2.88
O
N
S
F
F
F
S
CH3
4.81
1.00
1.00
2.95
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

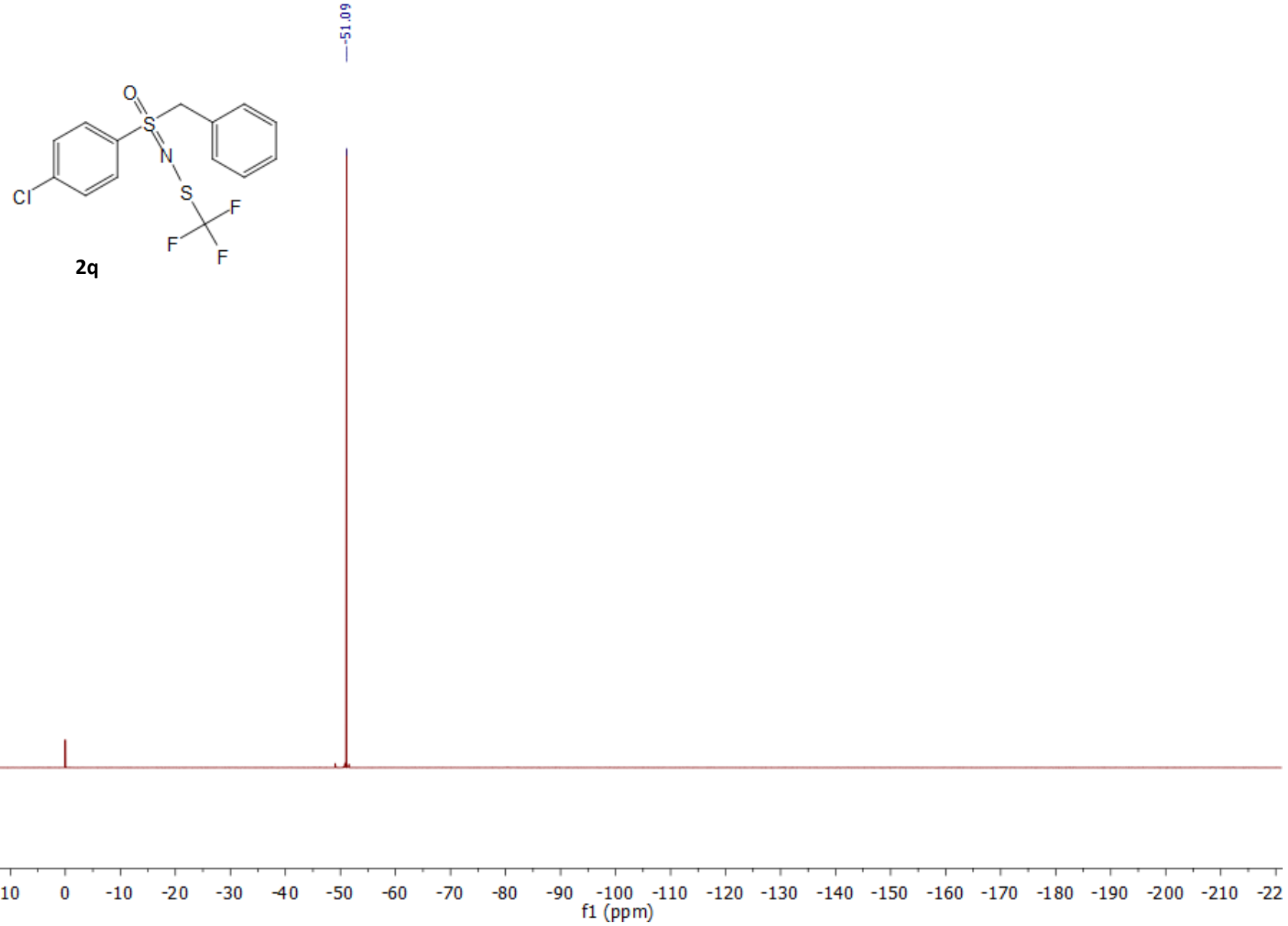
2p


-51.76
O
N
S
F
F
F
S
CH3
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

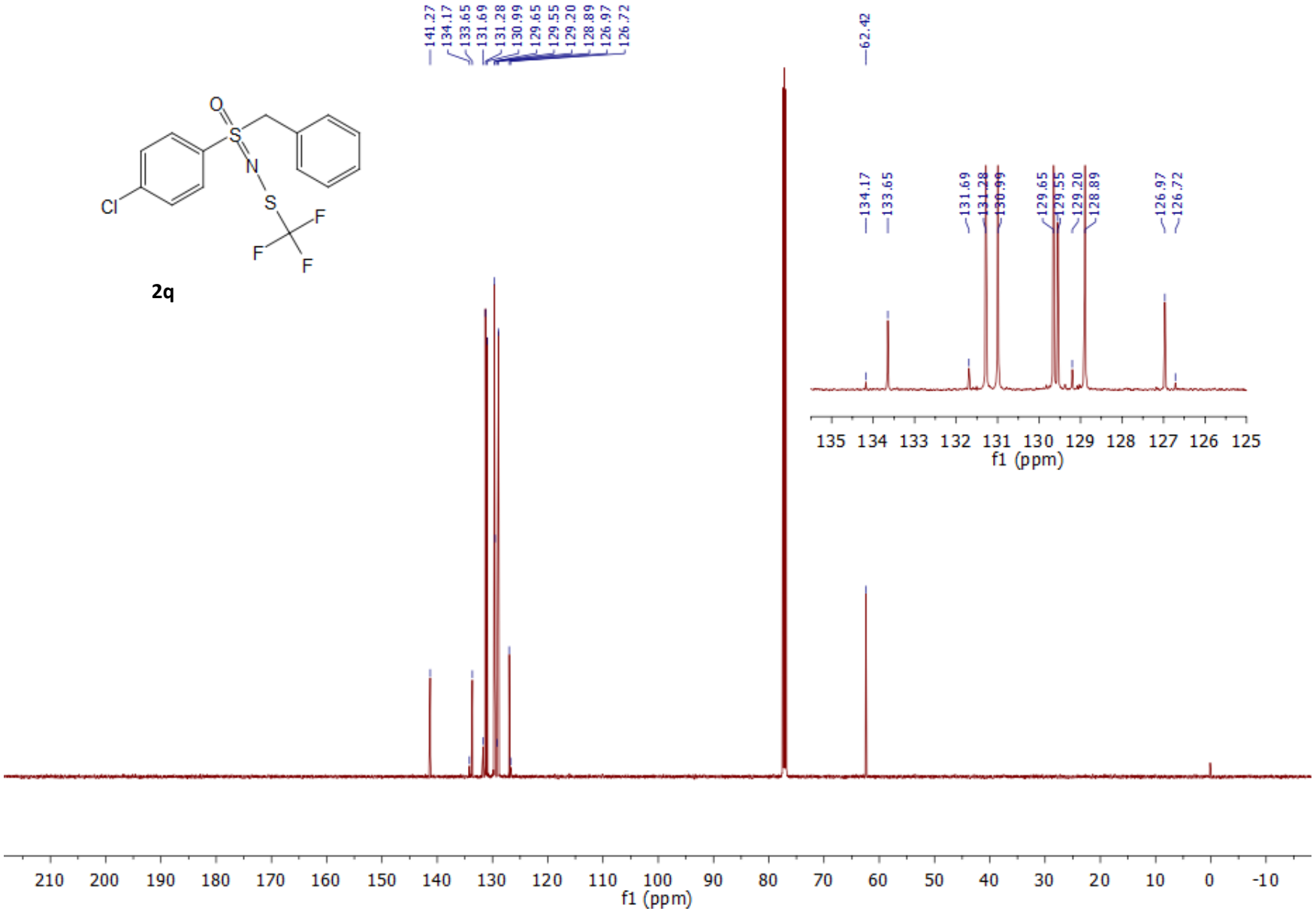
2p

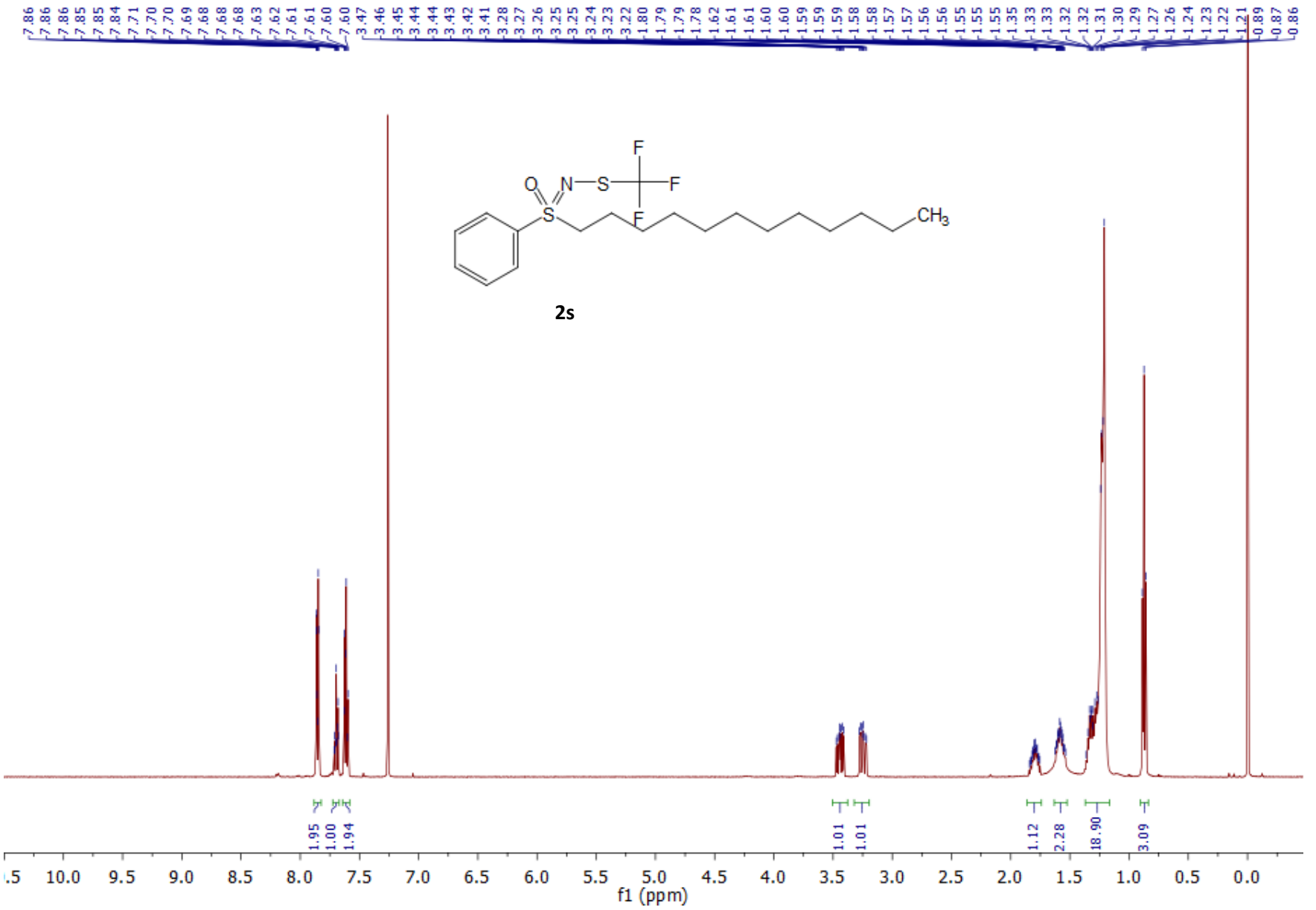

O
N
S
F
F
F
S
CH3
2p
134.30
131.81
130.98
129.81
129.33
126.84
60.58
37.47
135 134 133 132 131 130 129 128 127 126
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

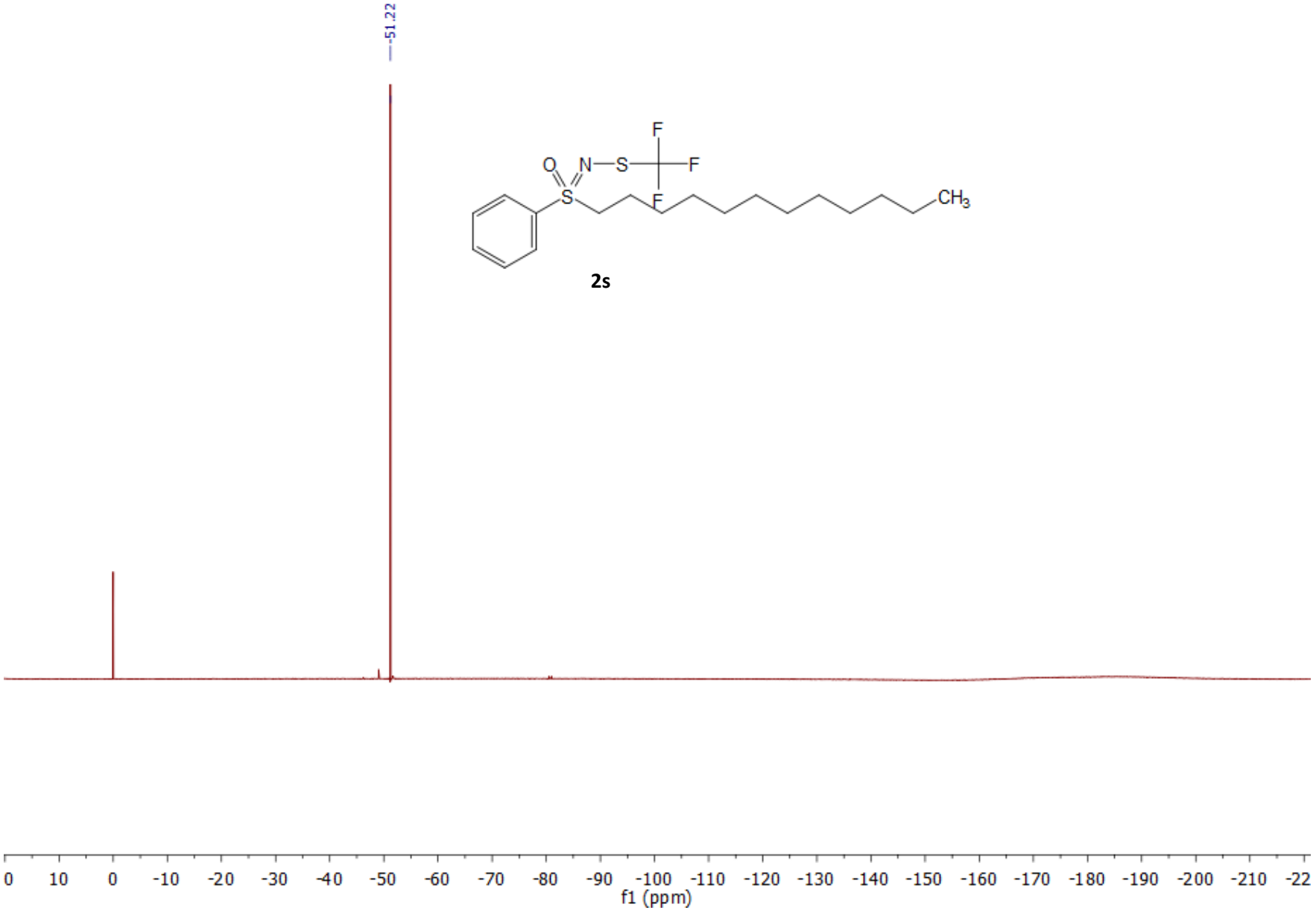

7.49 7.49 7.48 7.47 7.47 7.45 7.44 7.44 7.43 7.42 7.35 7.35 7.34 7.34 7.33 7.32 7.32 7.32 7.27 7.27 7.26 7.26 7.25 7.24 7.24 7.03 7.03 7.01 7.01
4.69 4.66 4.51 4.48
O
S
N
S
O
F
F
F
Cl
2q
1.97 1.96 1.01 2.39 1.94
1.00 0.99
f1 (ppm)


-51.09
O
S
N
S
F
F
F
Cl
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

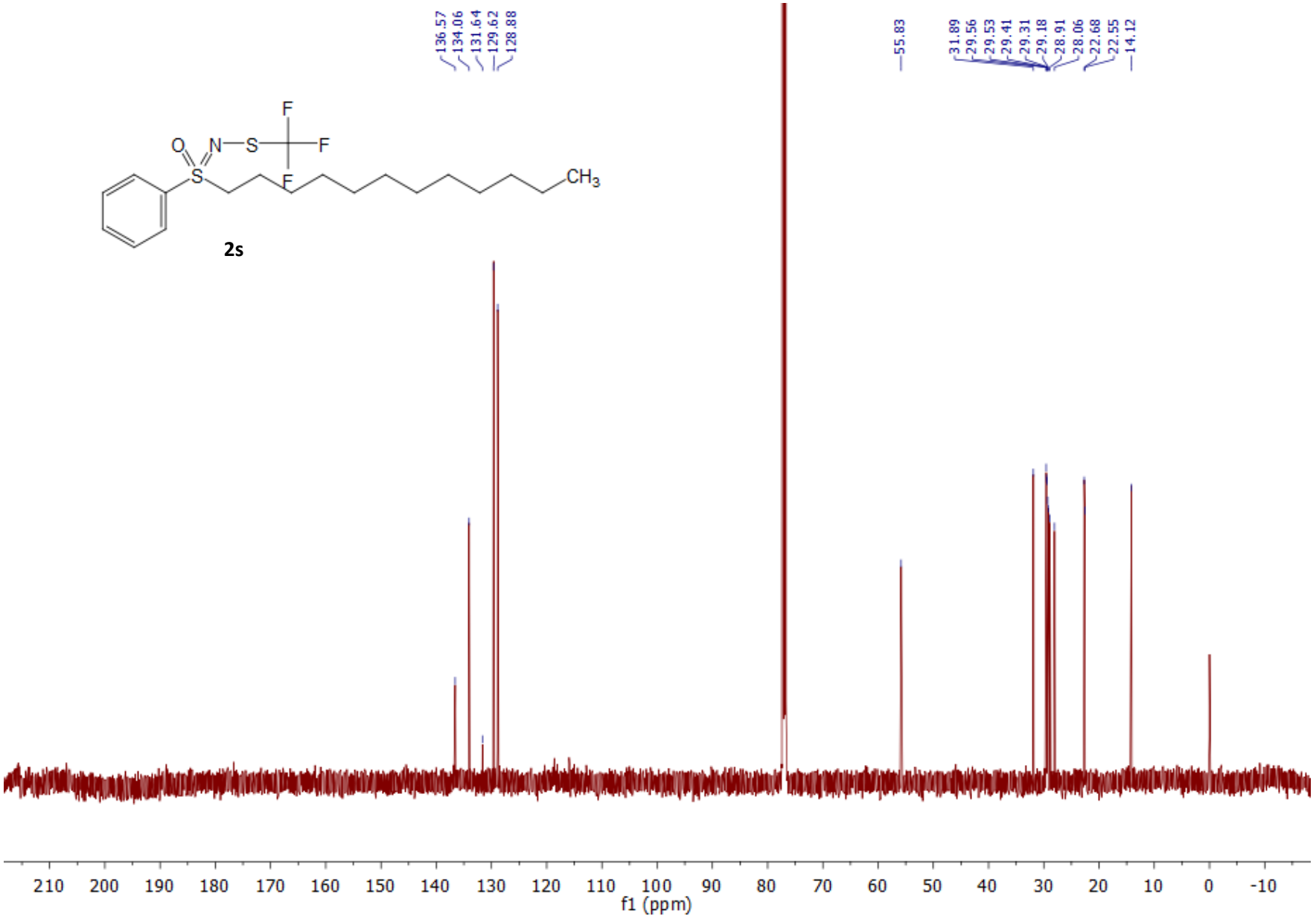
2q

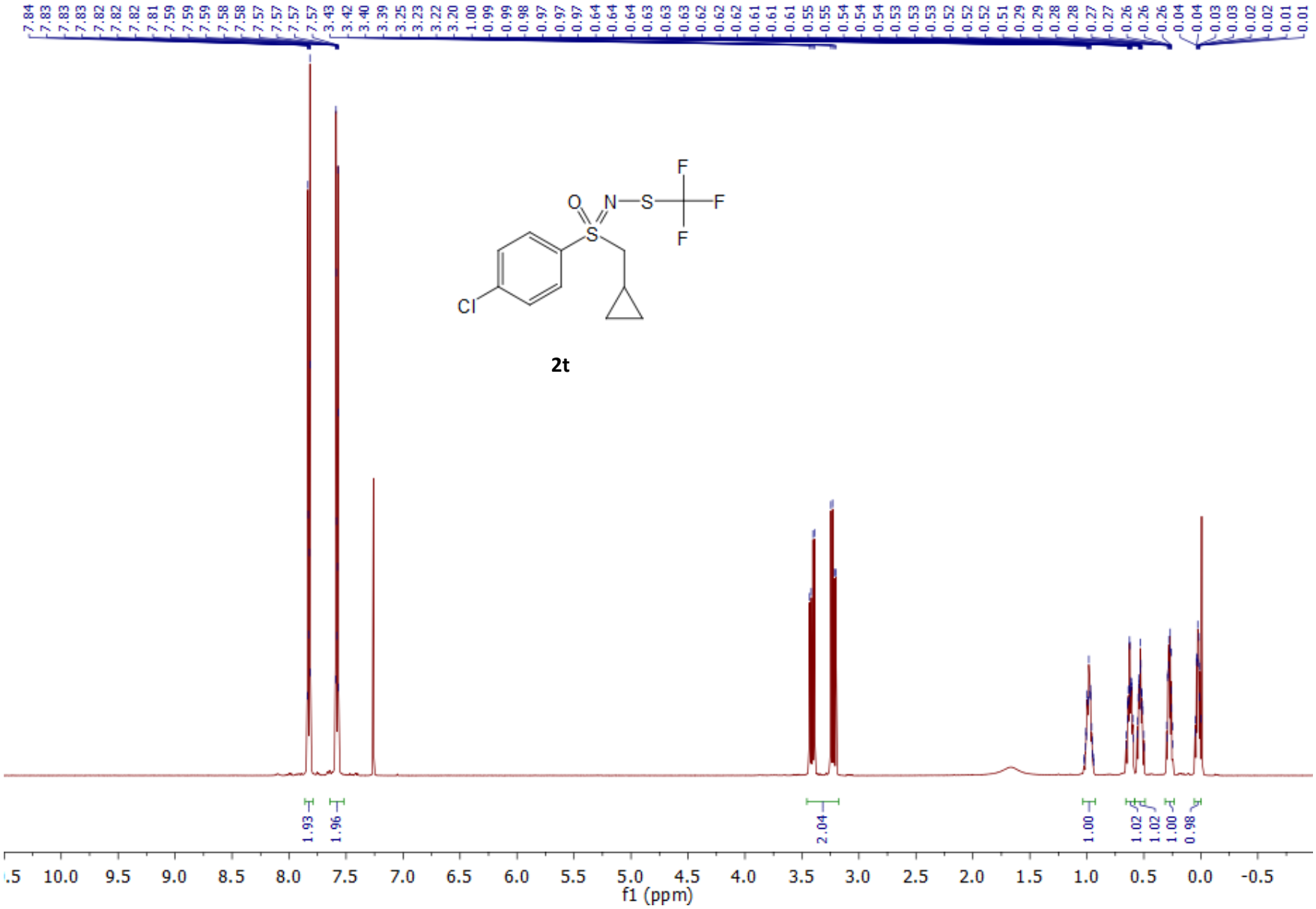

141.27
134.17
133.65
131.69
131.28
130.99
129.65
129.55
129.20
128.89
126.97
126.72
62.42
O
S
N
S
F
F
F
Cl
2q
134.17
133.65
131.69
131.28
130.99
129.65
129.55
129.20
128.89
126.97
126.72
135 134 133 132 131 130 129 128 127 126 125
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


F
O
N
S
F
S
F
CH3
2s
1.95
1.00
1.94
1.01
1.01
1.12
2.28
18.90
3.09
f1 (ppm)

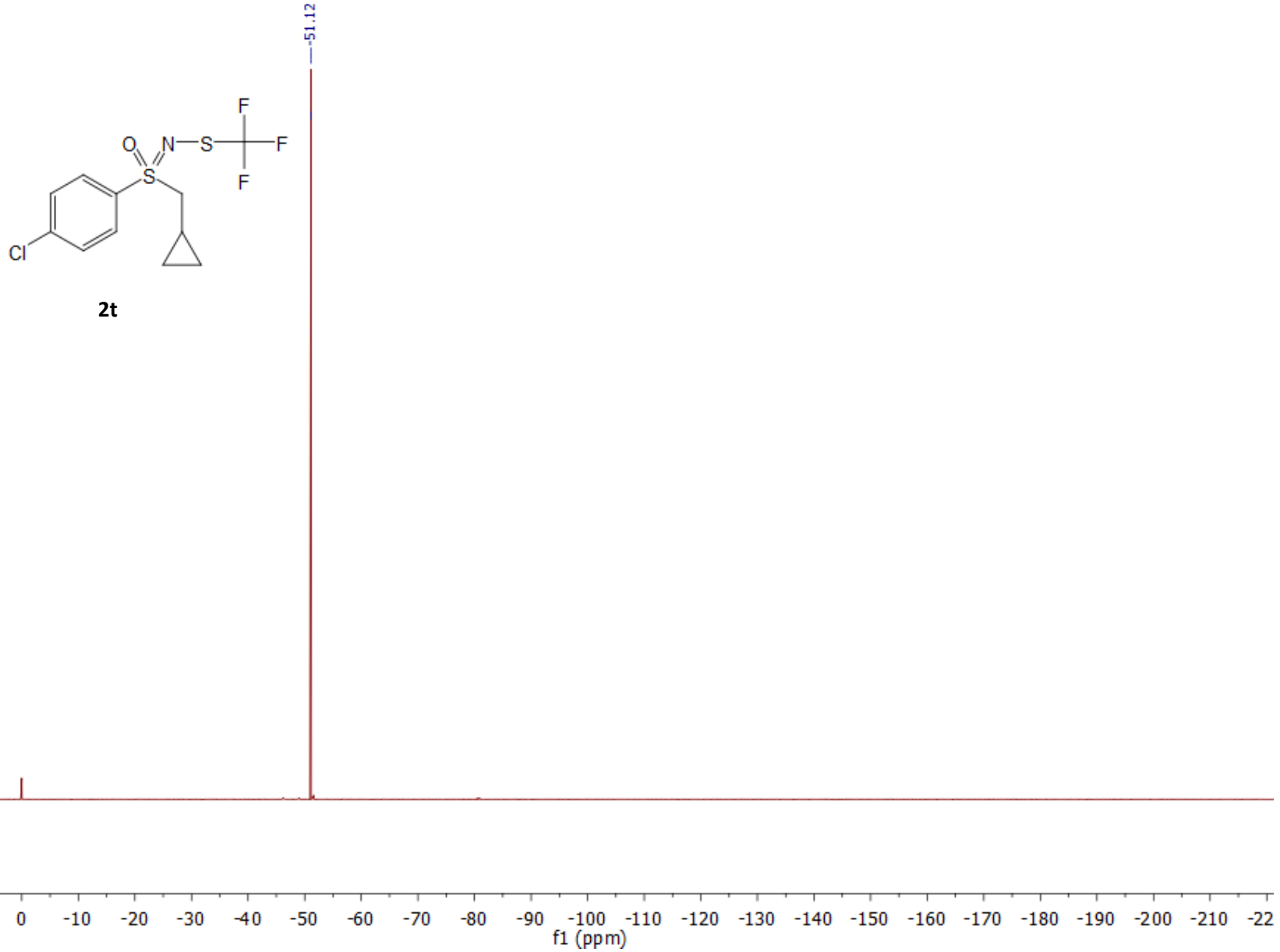

-51.22
F
O
N
S
F
S
F
CH3
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

2s

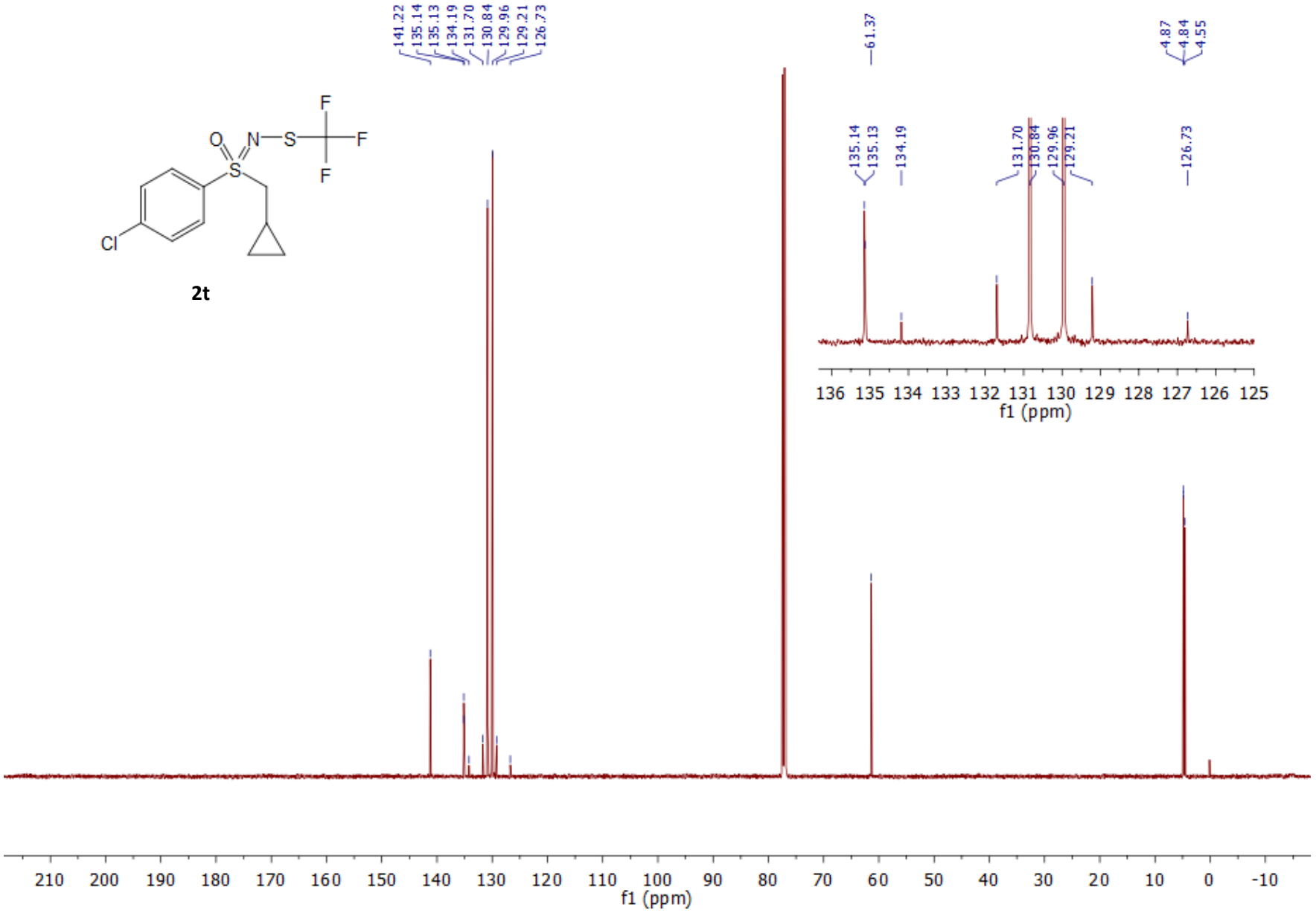

136.57
134.06
131.64
129.62
128.88
55.83
31.89
29.56
29.53
29.41
29.31
29.18
28.91
28.06
22.68
22.55
14.12
O
N
S
F
F
F
S
CH3
2s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

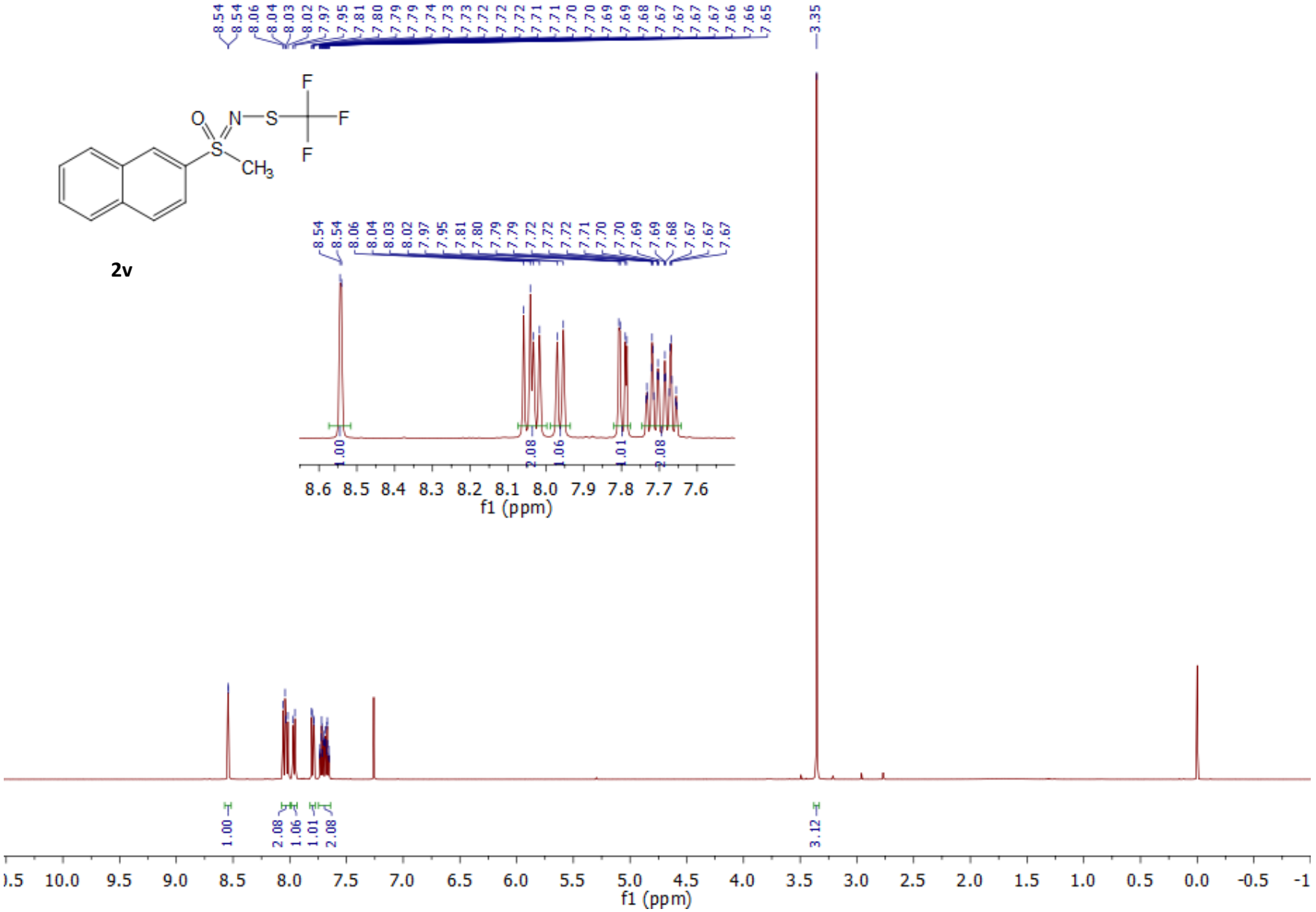

7.84 7.83 7.83 7.83 7.82 7.82 7.82 7.81 7.59 7.59 7.59 7.58 7.58 7.57 7.57 7.57 7.57 3.43 3.42 3.40 3.39 3.25 3.23 3.22 3.20 1.00 0.99 0.99 0.98 0.97 0.97 0.97 0.64 0.64 0.64 0.63 0.63 0.63 0.62 0.62 0.62 0.61 0.61 0.61 0.55 0.55 0.54 0.54 0.54 0.53 0.53 0.53 0.52 0.52 0.52 0.51 0.29 0.29 0.28 0.28 0.27 0.27 0.26 0.26 0.26 0.04 0.04 0.03 0.03 0.02 0.02 0.01 0.01
O
N
S
F
F
F
S
Cl
1.93
1.96
2.04
1.00
1.02
1.02
1.00
0.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

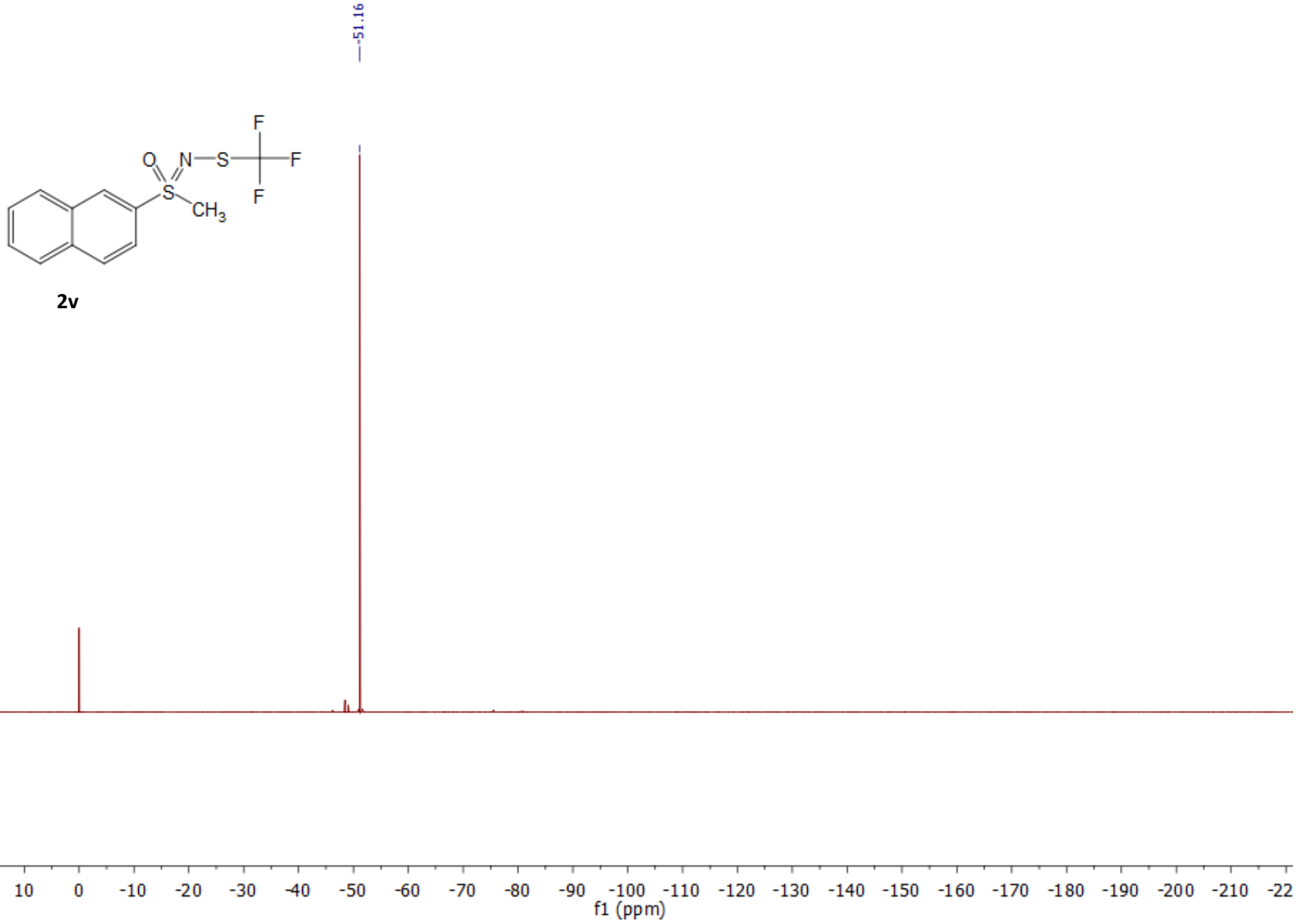
2t


-51.12
F
O
N
S
F
S
F
Cl
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

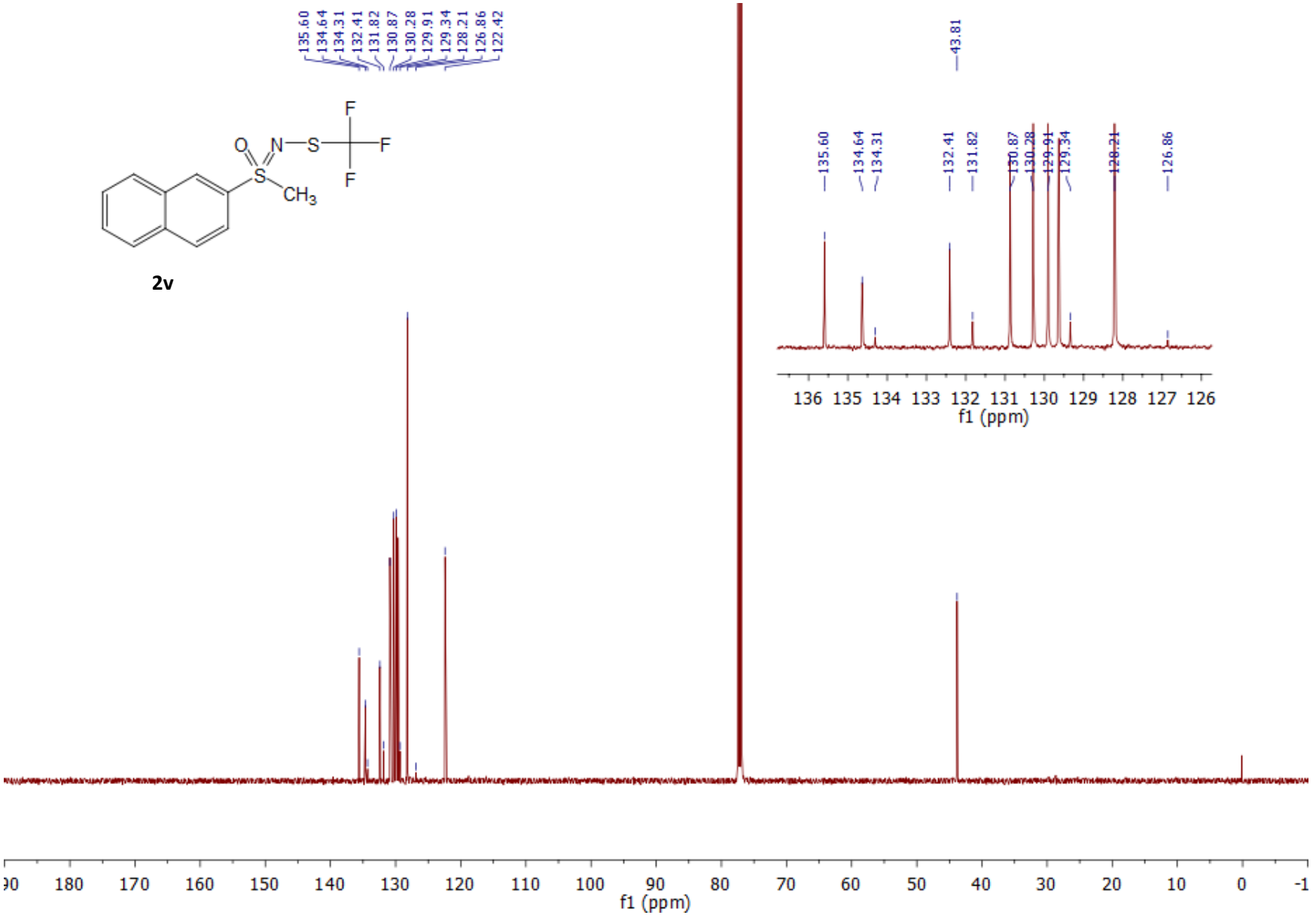
2t

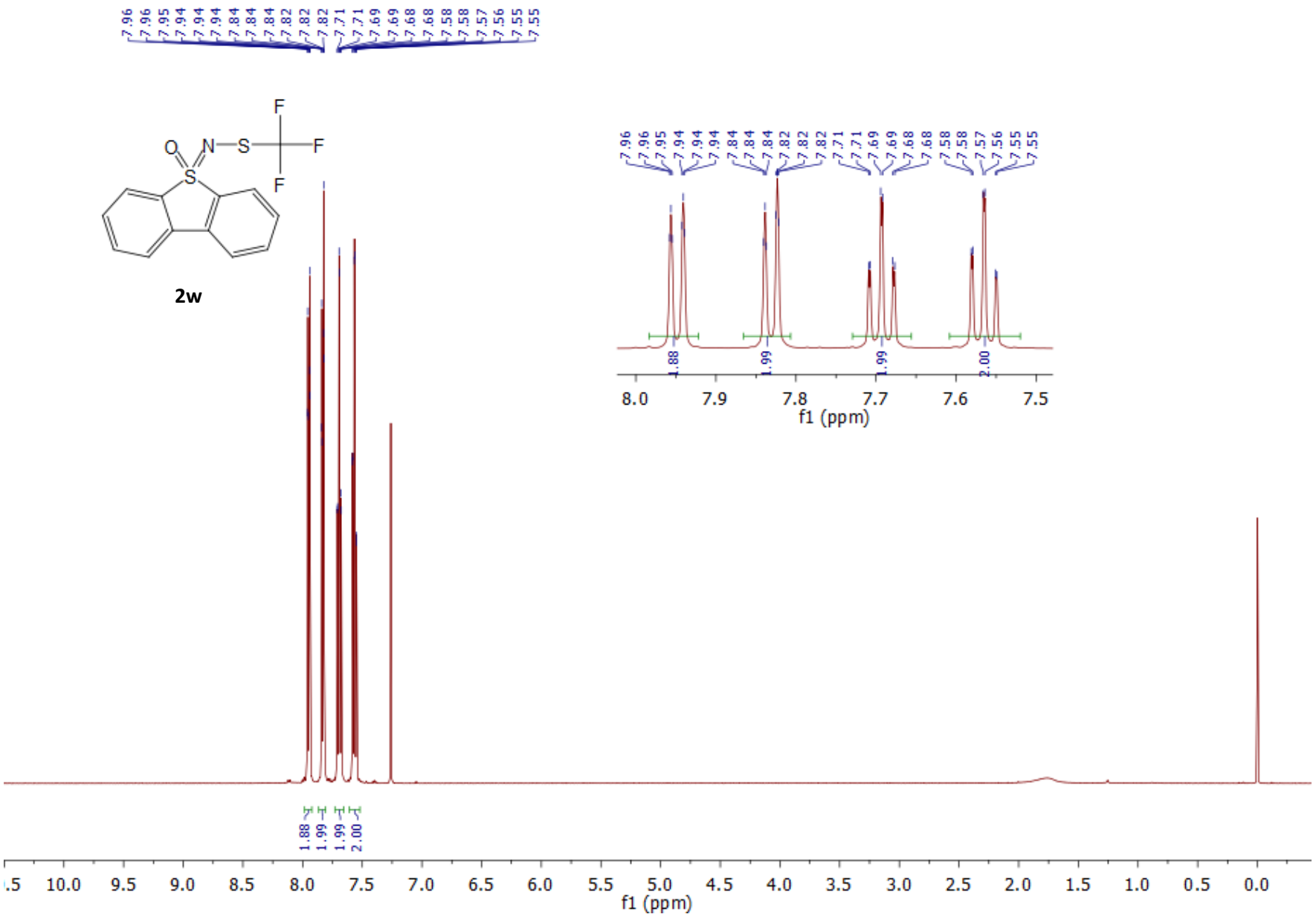

141.22
135.14
135.13
134.19
131.70
130.84
129.96
129.21
126.73
61.37
4.87
4.84
4.55
F
O
N
S
F
S
F
Cl
2t
135.14
135.13
134.19
131.70
130.84
129.96
129.21
126.73
136 135 134 133 132 131 130 129 128 127 126 125
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


F
O
N
S
F
S
F
CH3
2v
8.54
8.54
8.06
8.04
8.03
8.02
7.97
7.95
7.81
7.80
7.79
7.79
7.74
7.73
7.73
7.72
7.72
7.72
7.71
7.71
7.70
7.70
7.69
7.69
7.68
7.67
7.67
7.67
7.67
7.66
7.66
7.65
3.35
1.00
2.08
1.06
1.01
2.08
8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6
f1 (ppm)
3.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


-51.16
F
O
N
S
F
S
F
CH3
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

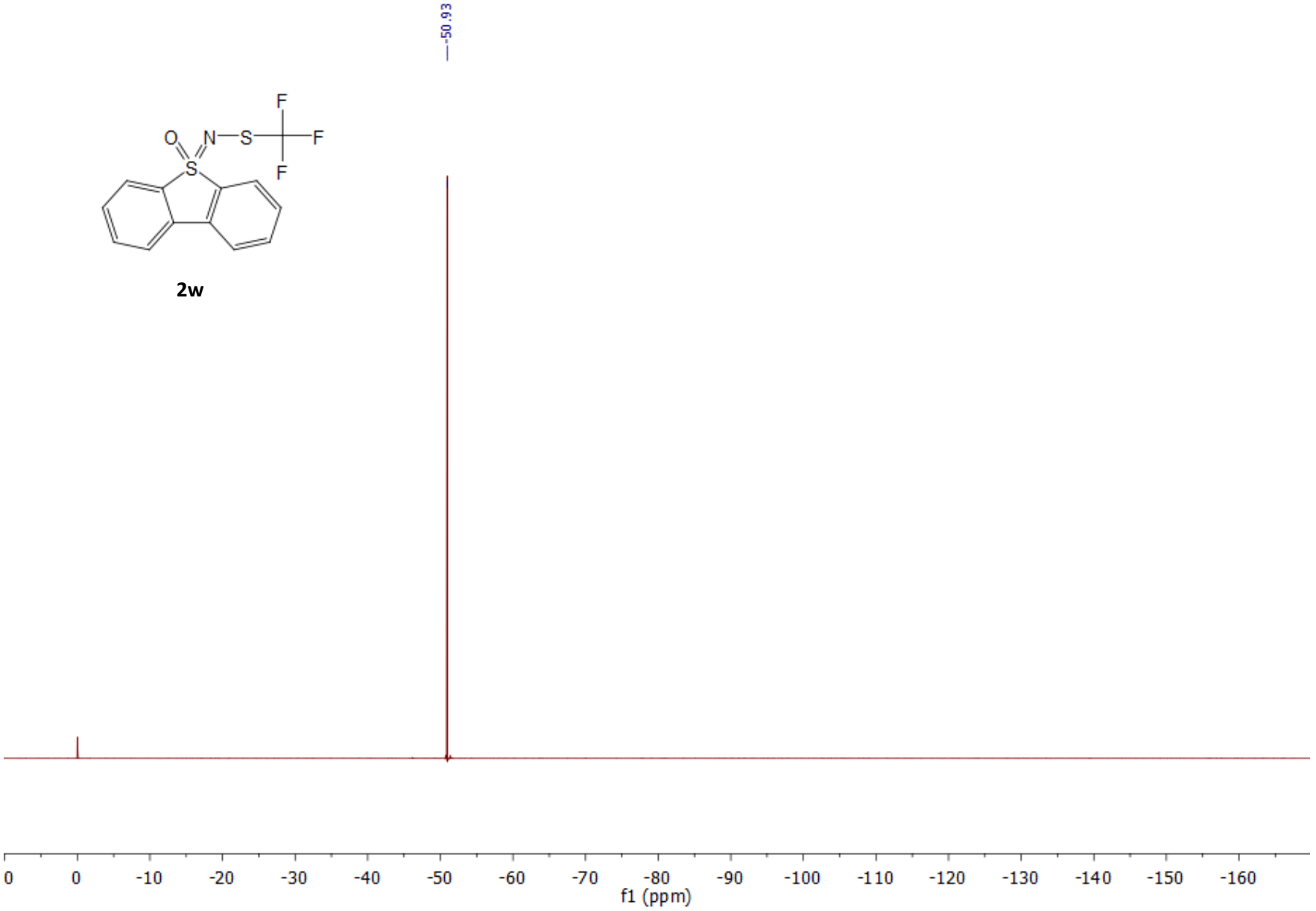
2v

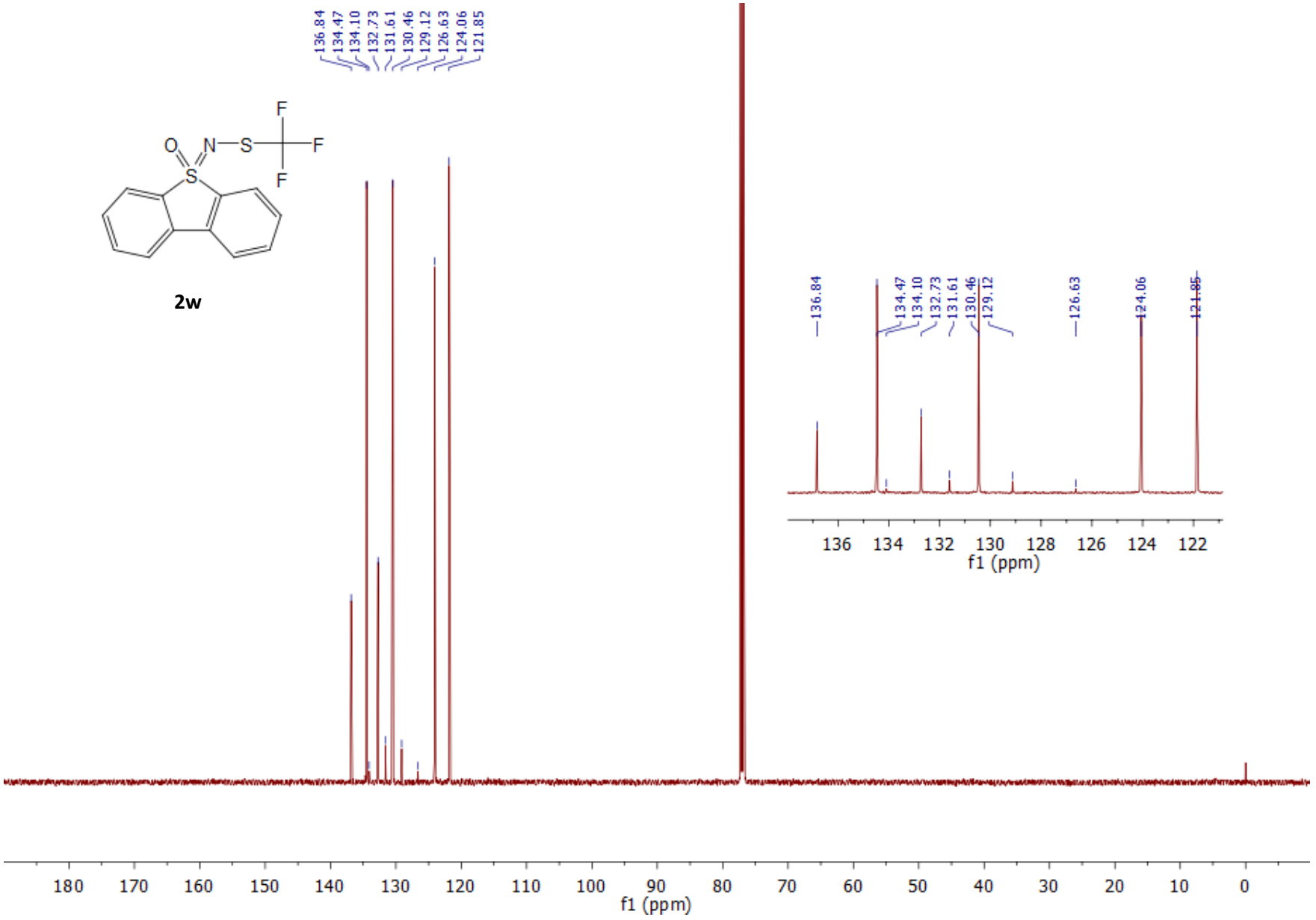

135.60
134.64
134.31
132.41
131.82
130.87
130.28
129.91
129.34
128.21
126.86
122.42
43.81
F
O
N
S
F
S
F
CH3
2v
135.60
134.64
134.31
132.41
131.82
130.87
130.28
129.91
129.34
128.21
126.86
136 135 134 133 132 131 130 129 128 127 126
f1 (ppm)
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

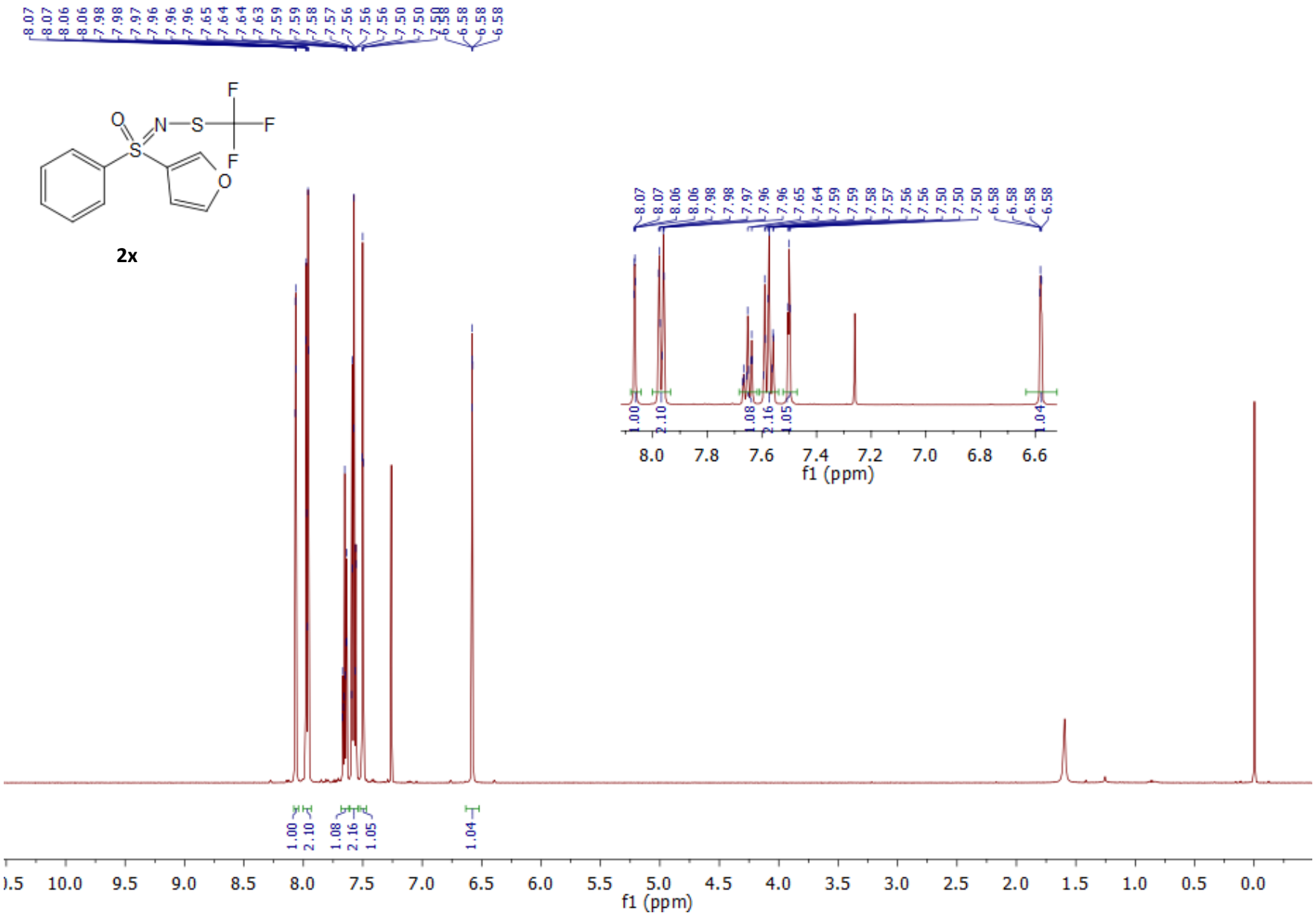

7.96 7.96 7.95 7.94 7.94 7.94 7.84 7.84 7.84 7.82 7.82 7.82 7.71 7.71 7.69 7.69 7.68 7.68 7.58 7.58 7.57 7.56 7.55 7.55
F
O
N
S
F
S
F
2w
7.96 7.96 7.95 7.94 7.94 7.94 7.84 7.84 7.84 7.82 7.82 7.82 7.71 7.71 7.69 7.69 7.68 7.68 7.58 7.58 7.57 7.56 7.55 7.55
1.88 1.99 1.99 2.00
8.0 7.9 7.8 7.7 7.6 7.5
f1 (ppm)
1.88 1.99 1.99 2.00
.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

O
N
S
F
F
F
S

2w

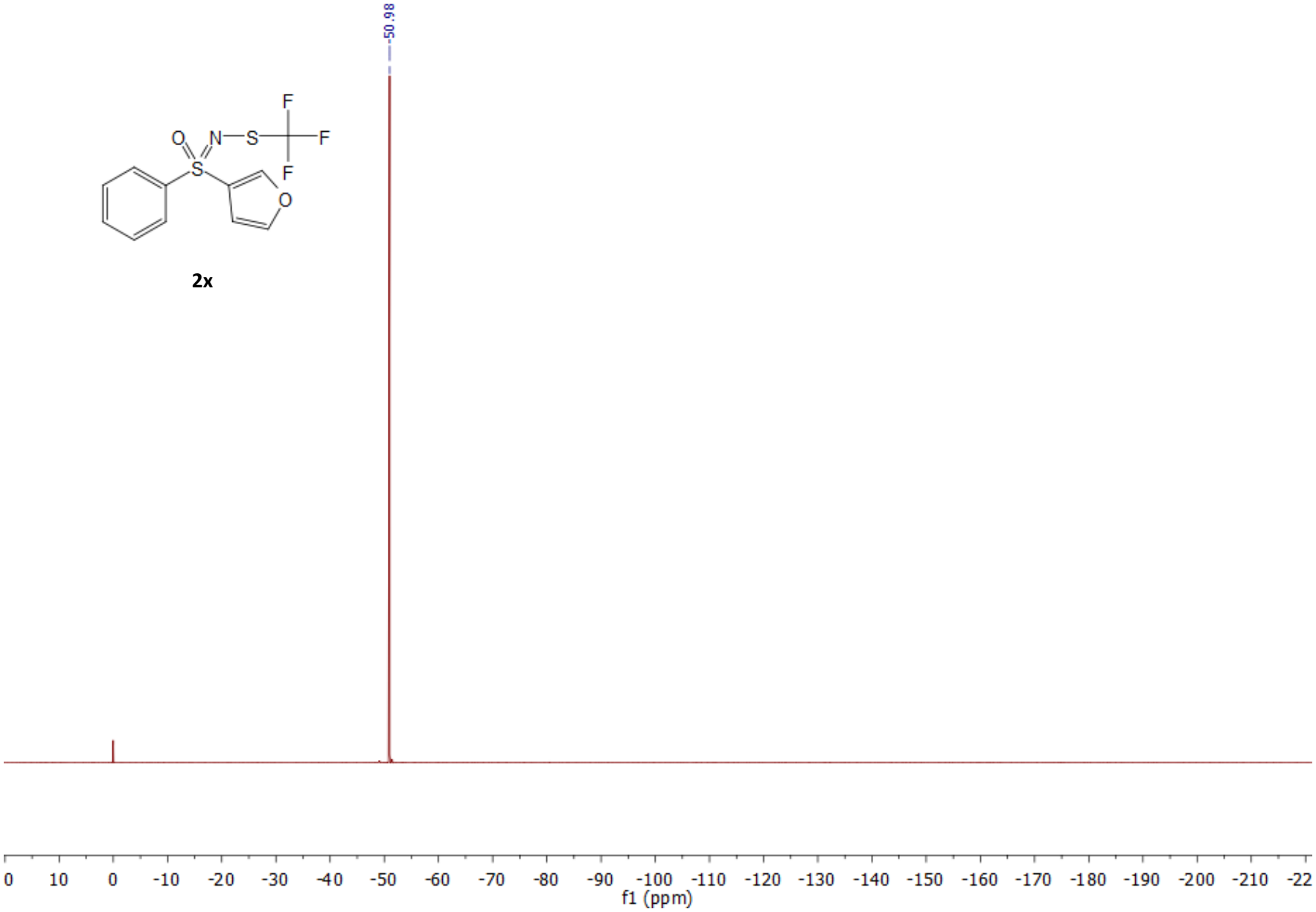

-50.93
0
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
f1 (ppm)

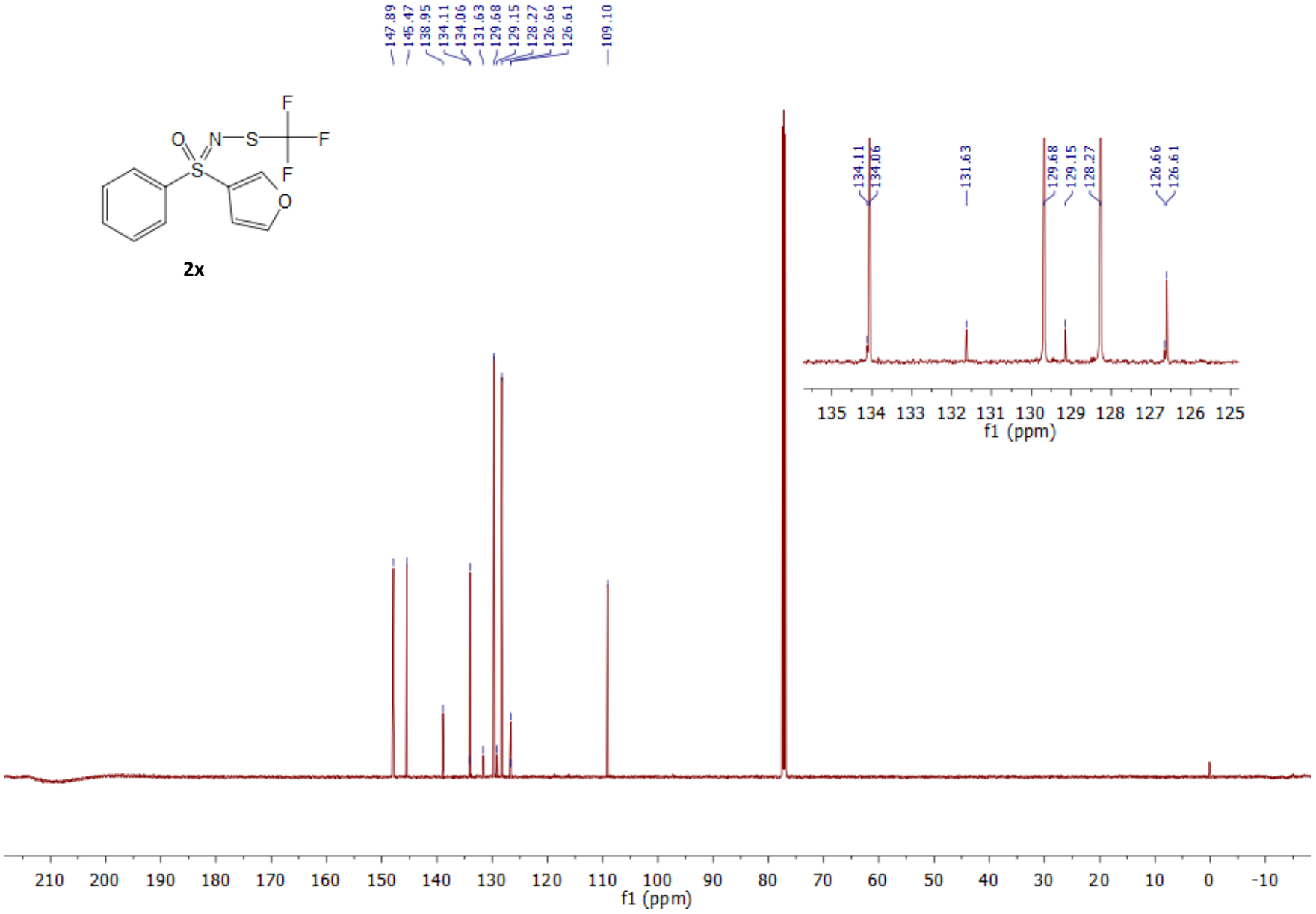

136.84
134.47
134.10
132.73
131.61
130.46
129.12
126.63
124.06
121.85
F
O
N
S
F
S
F
2w
136.84
134.47
134.10
132.73
131.61
130.46
129.12
126.63
124.06
121.85
136
134
132
130
128
126
124
122
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

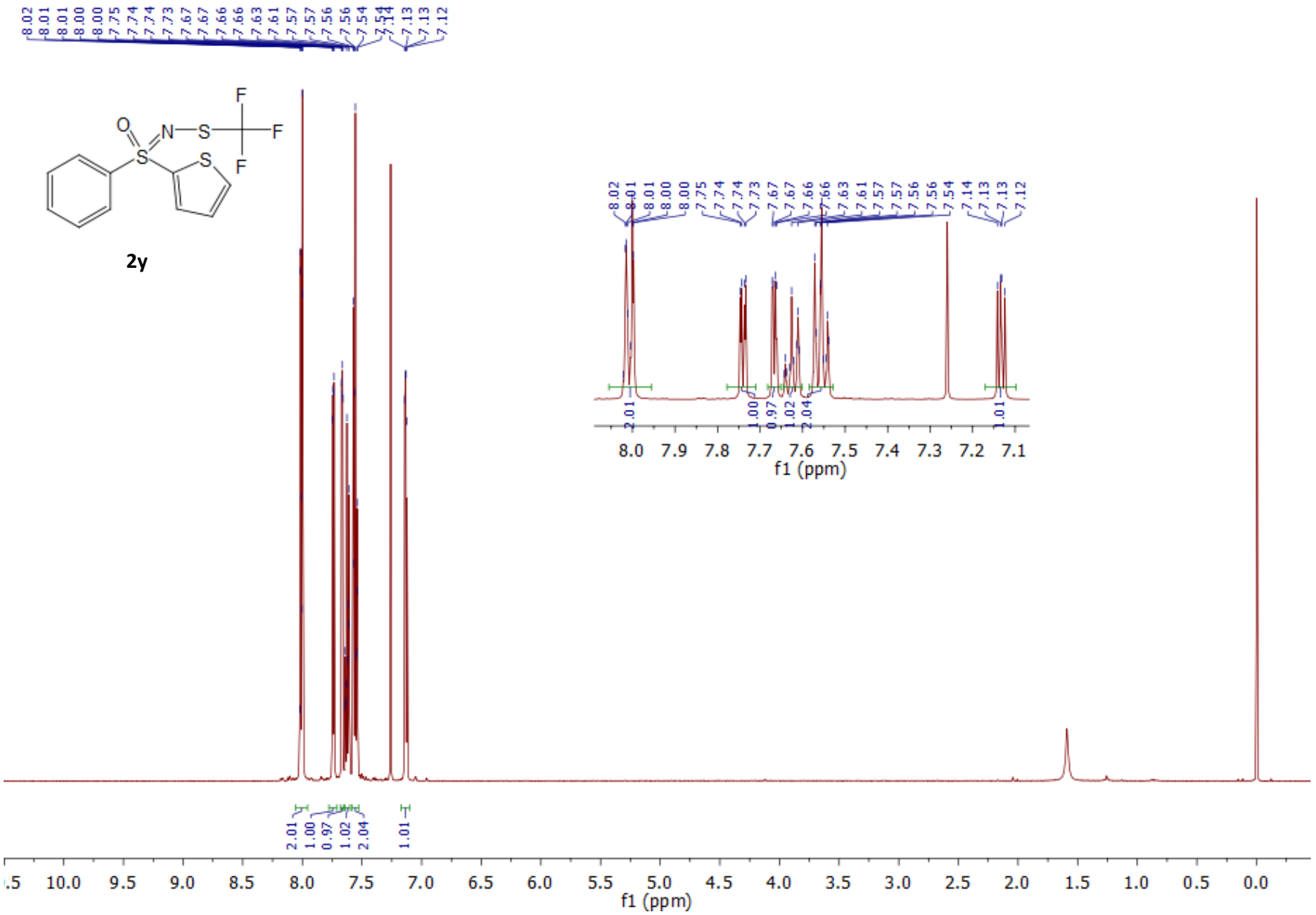

8.07 8.07 8.06 8.06 7.98 7.98 7.97 7.96 7.96 7.96 7.65 7.64 7.64 7.63 7.59 7.59 7.58 7.57 7.56 7.56 7.56 7.50 7.50 7.50 6.58 6.58 6.58
F
O
N
S
F
S
F
O
2x
1.00 2.10 1.08 2.16 1.05 1.04
f1 (ppm)

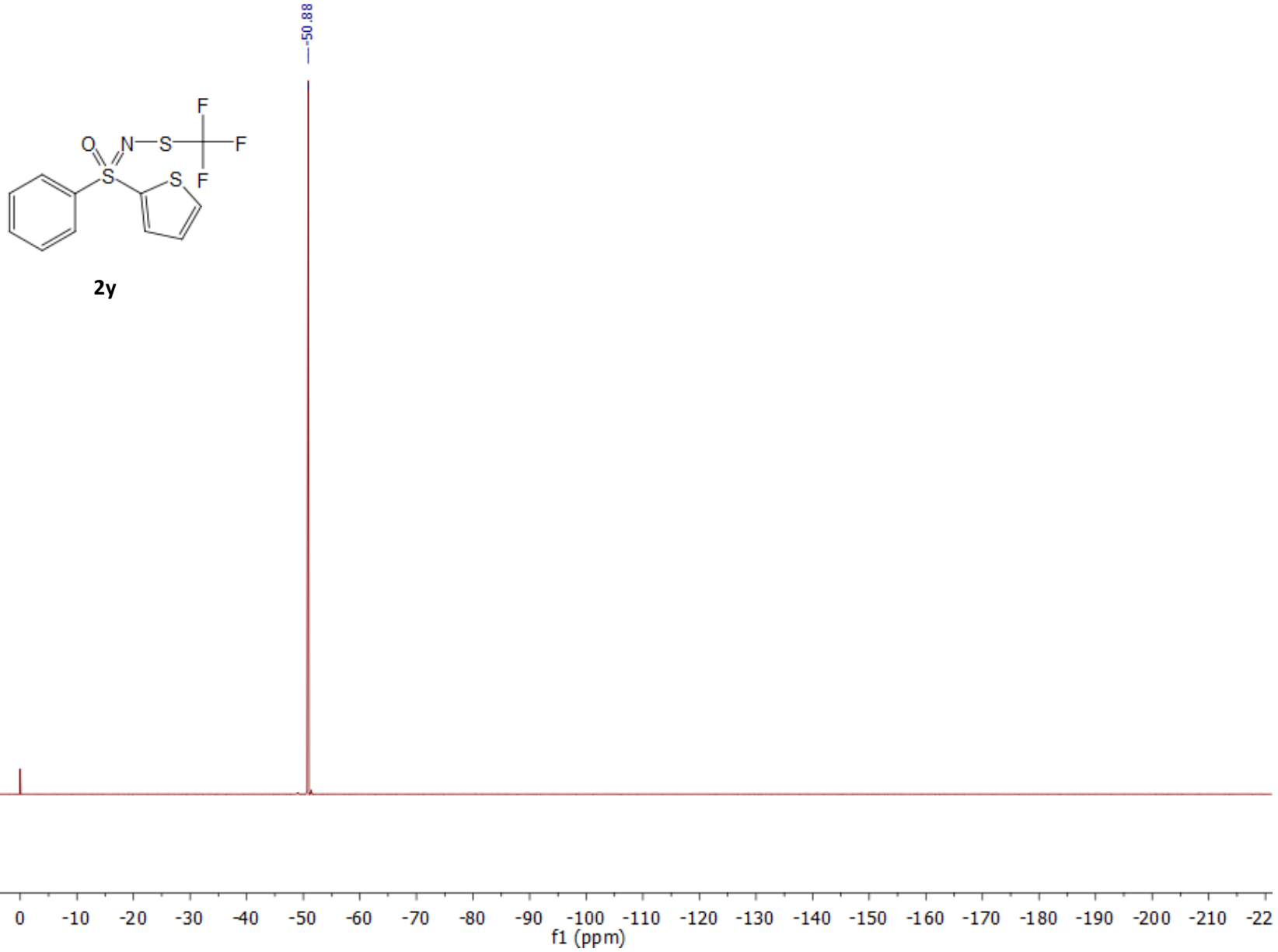
O
N
S
F
F
F
S
O

2x

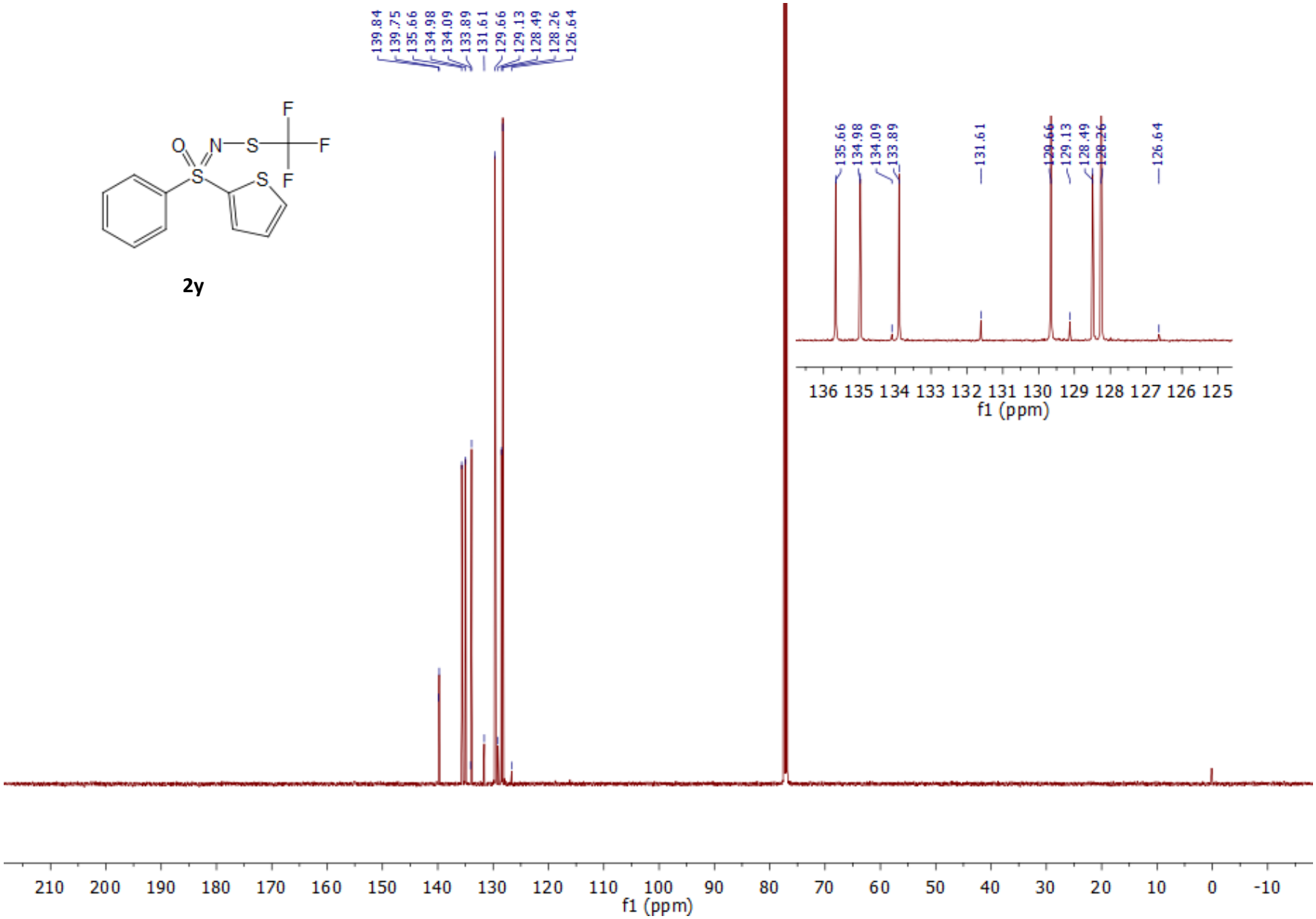

-50.98
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

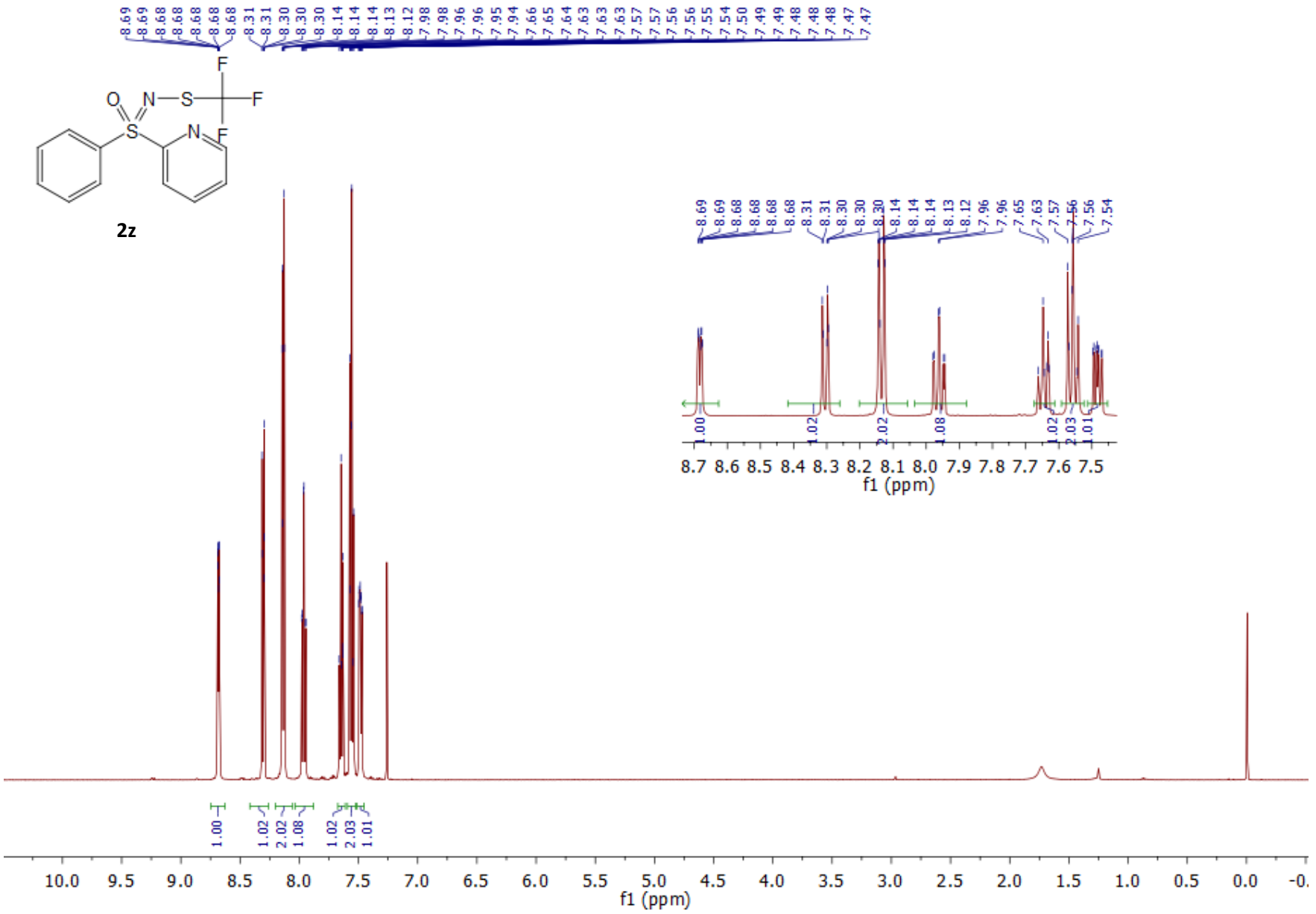

147.89
145.47
138.95
134.11
134.06
131.63
129.68
129.15
128.27
126.66
126.61
109.10
F
O
N
S
F
F
S
O
2x
134.11
134.06
131.63
129.68
129.15
128.27
126.66
126.61
135 134 133 132 131 130 129 128 127 126 125
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.02 8.01 8.01 8.00 8.00 7.75 7.74 7.74 7.73 7.67 7.67 7.66 7.66 7.63 7.61 7.57 7.57 7.56 7.56 7.54 7.14 7.13 7.13 7.12
O
N
S
S
S
F
F
F
2y
2.01 1.00 0.97 1.02 2.04 1.01
f1 (ppm)


-50.88
F
O
N
S
F
S
S
F
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

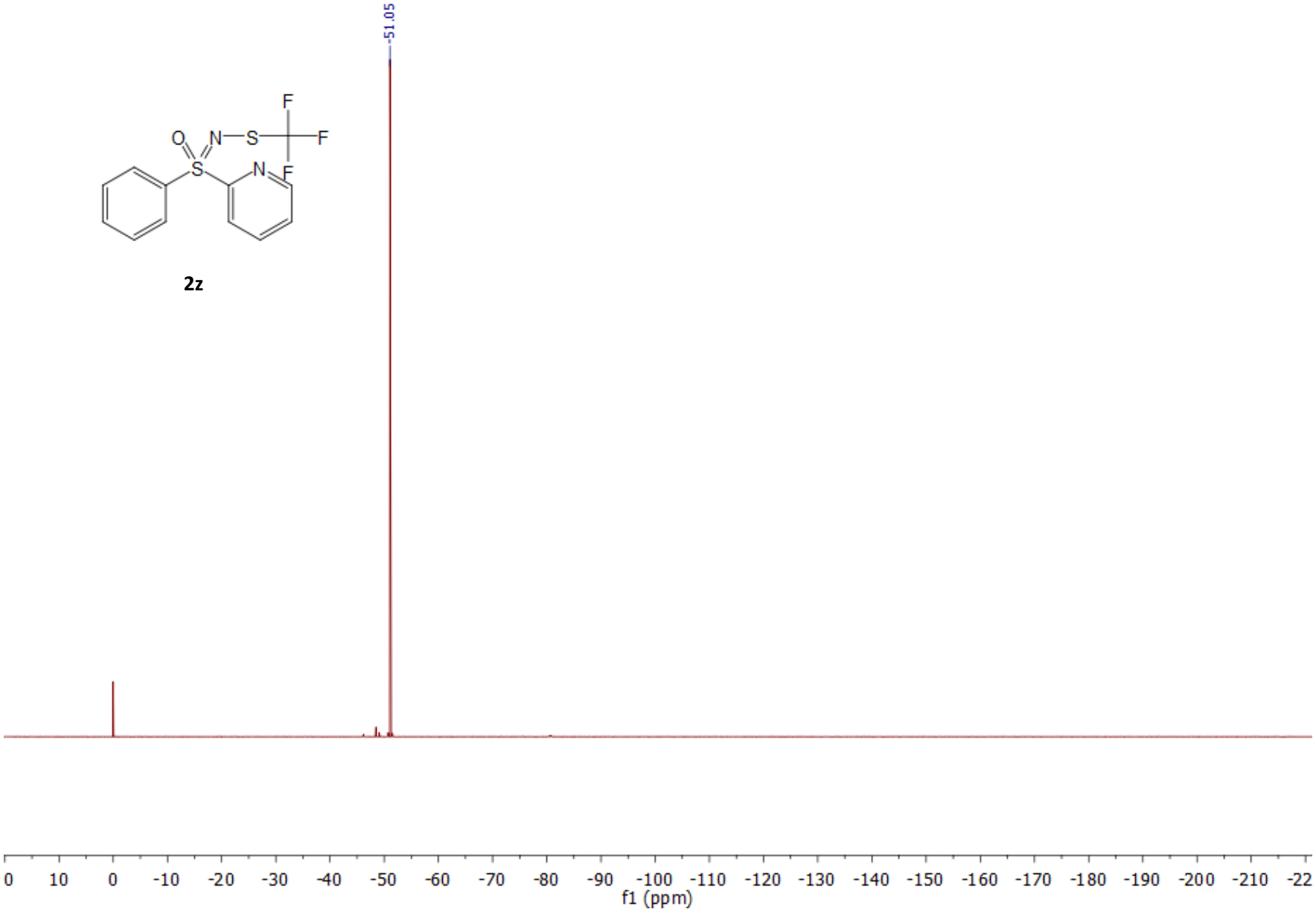
2y

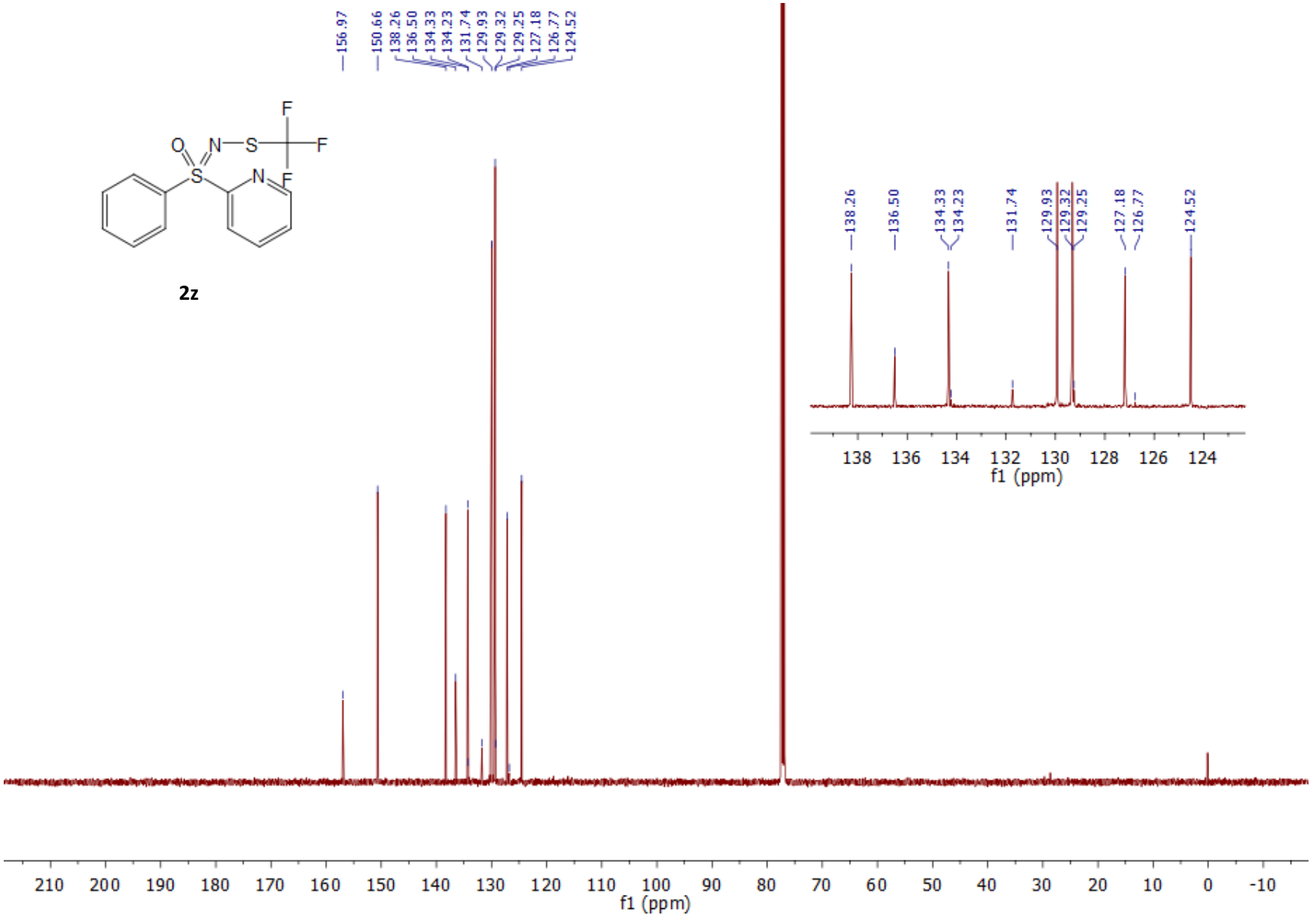

139.84
139.75
135.66
134.98
134.09
133.89
131.61
129.66
129.13
128.49
128.26
126.64
F
O
N
S
F
S
S
F
2y
135.66
134.98
134.09
133.89
131.61
129.66
129.13
128.49
128.26
126.64
136 135 134 133 132 131 130 129 128 127 126 125
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

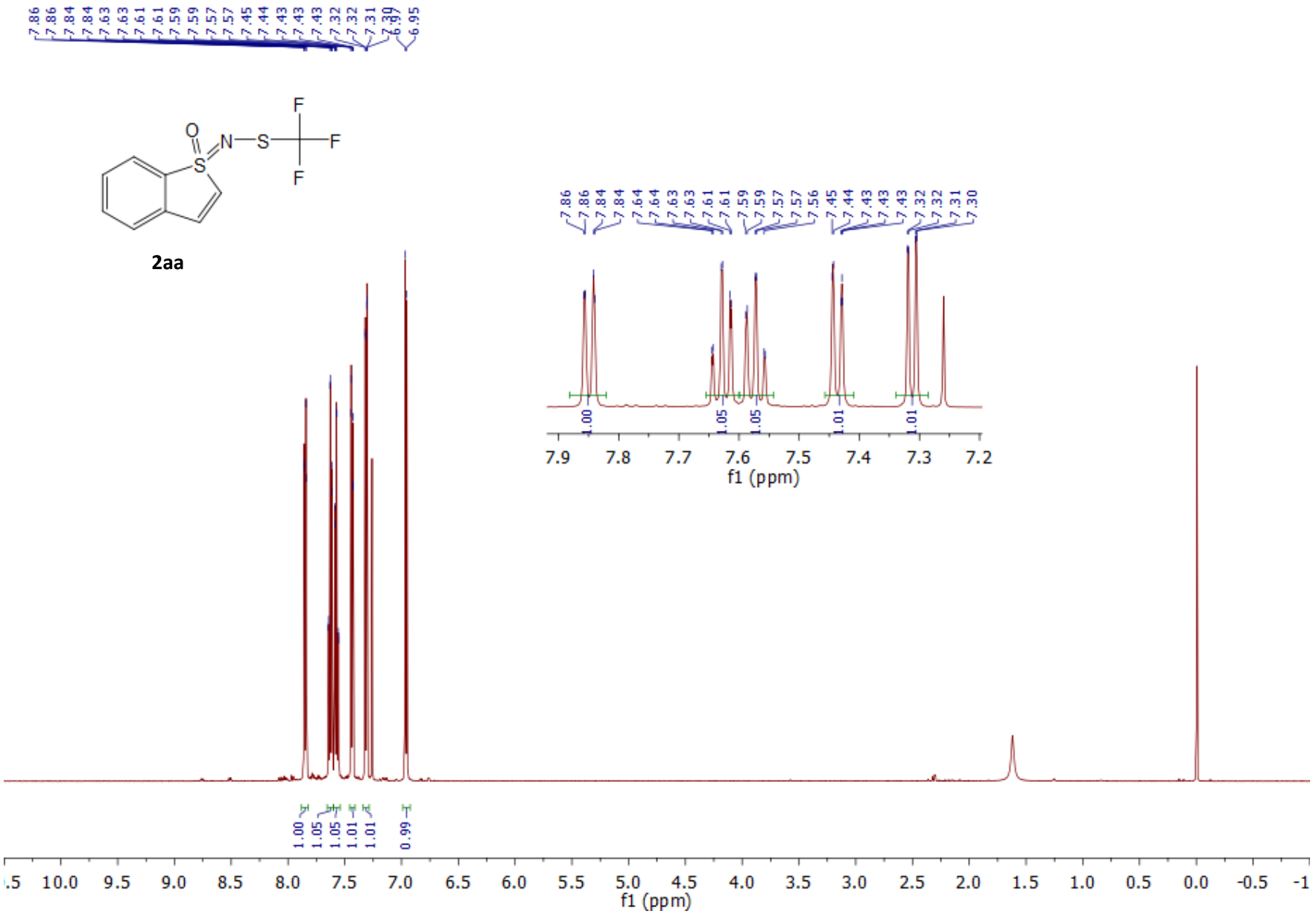

F
O
N
S
F
S
N
F
2z
8.69 8.69 8.68 8.68 8.68 8.68 8.31 8.31 8.30 8.30 8.30 8.14 8.14 8.14 8.13 8.12 7.98 7.98 7.96 7.96 7.95 7.94 7.66 7.65 7.64 7.63 7.63 7.63 7.57 7.57 7.56 7.56 7.55 7.54 7.50 7.49 7.49 7.48 7.48 7.48 7.47 7.47
1.00 1.02 2.02 1.08 1.02 2.03 1.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
8.69 8.69 8.68 8.68 8.68 8.68 8.31 8.31 8.30 8.30 8.30 8.14 8.14 8.14 8.13 8.12 7.96 7.96 7.65 7.63 7.57 7.56 7.56 7.54
1.00 1.02 2.02 1.08 1.02 2.03 1.01
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
f1 (ppm)

O
N
S
F
F
S
N
F

2z

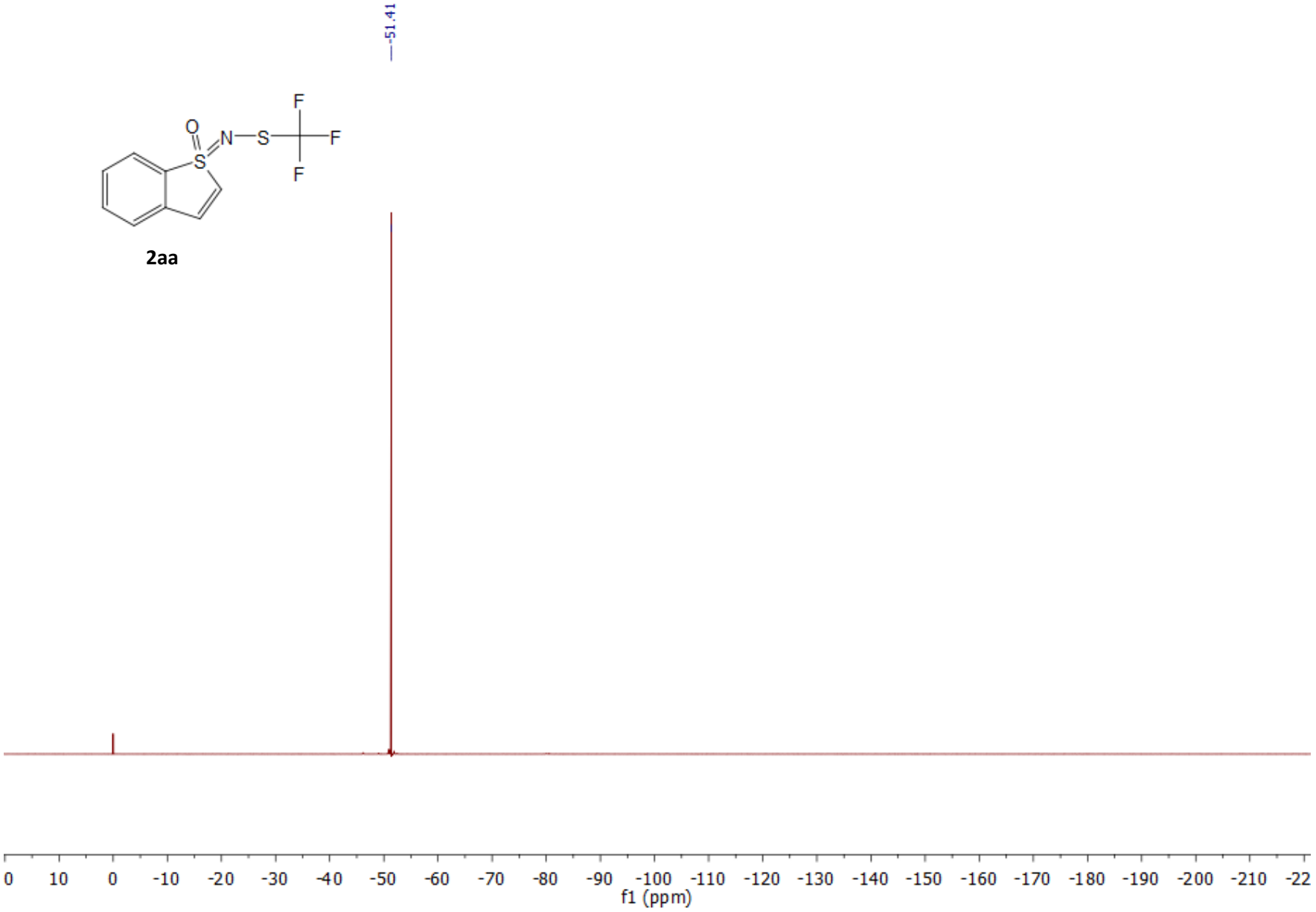

-51.05
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


156.97
150.66
138.26
136.50
134.33
134.23
131.74
129.93
129.32
129.25
127.18
126.77
124.52
F
O
N
S
F
S
N
F
2z
f1 (ppm)


7.86
7.86
7.84
7.84
7.63
7.63
7.61
7.61
7.59
7.59
7.57
7.57
7.45
7.44
7.43
7.43
7.43
7.32
7.32
7.31
6.95
O
N
S
S
F
F
F
2aa
7.86
7.86
7.84
7.84
7.64
7.64
7.63
7.63
7.61
7.61
7.59
7.59
7.57
7.57
7.56
7.45
7.44
7.43
7.43
7.43
7.32
7.32
7.31
7.30
1.00
1.05
1.05
1.01
1.01
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
1.00
1.05
1.05
1.01
1.01
0.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

O
N
S
F
F
F
S

2aa


-51.41
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
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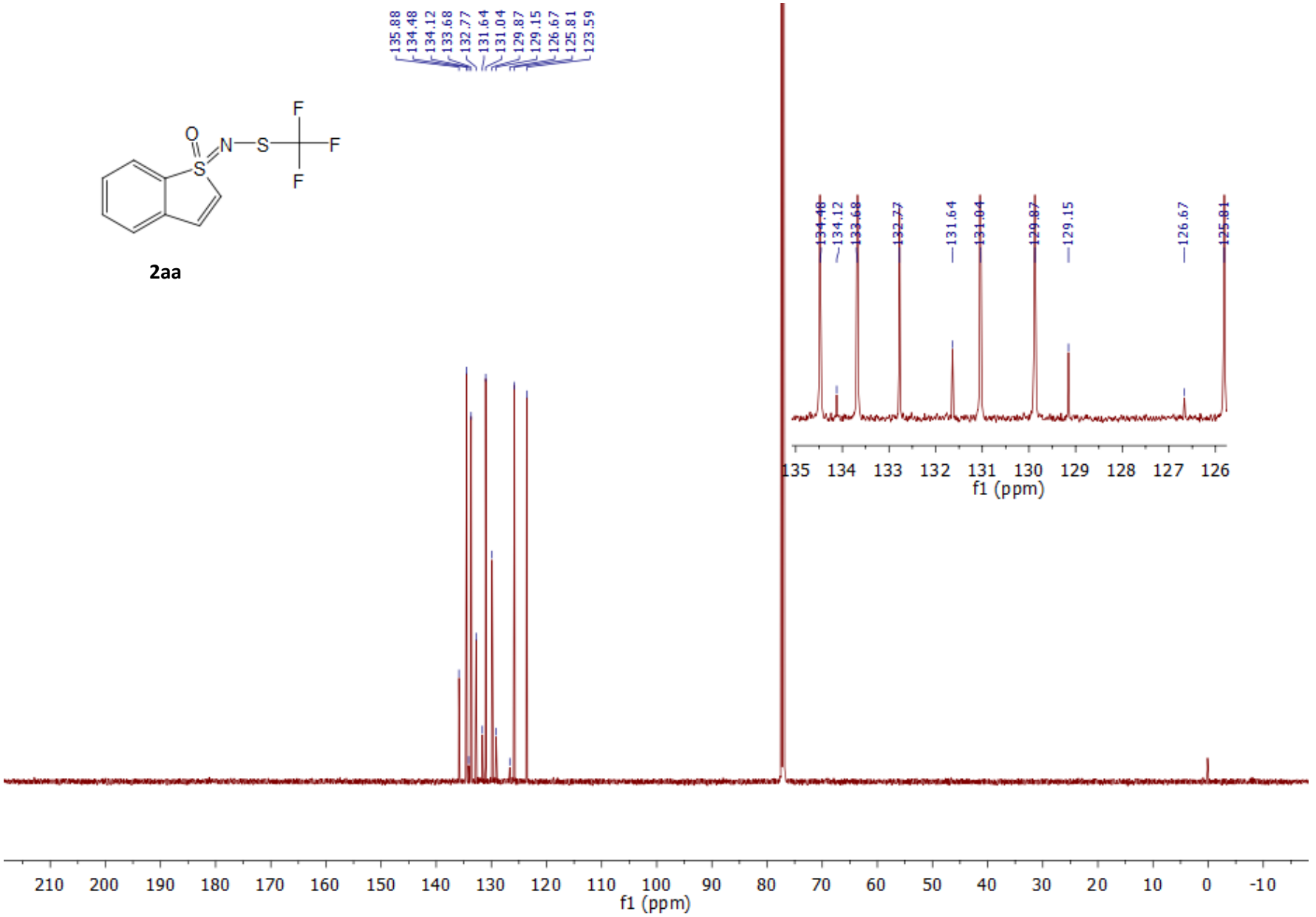
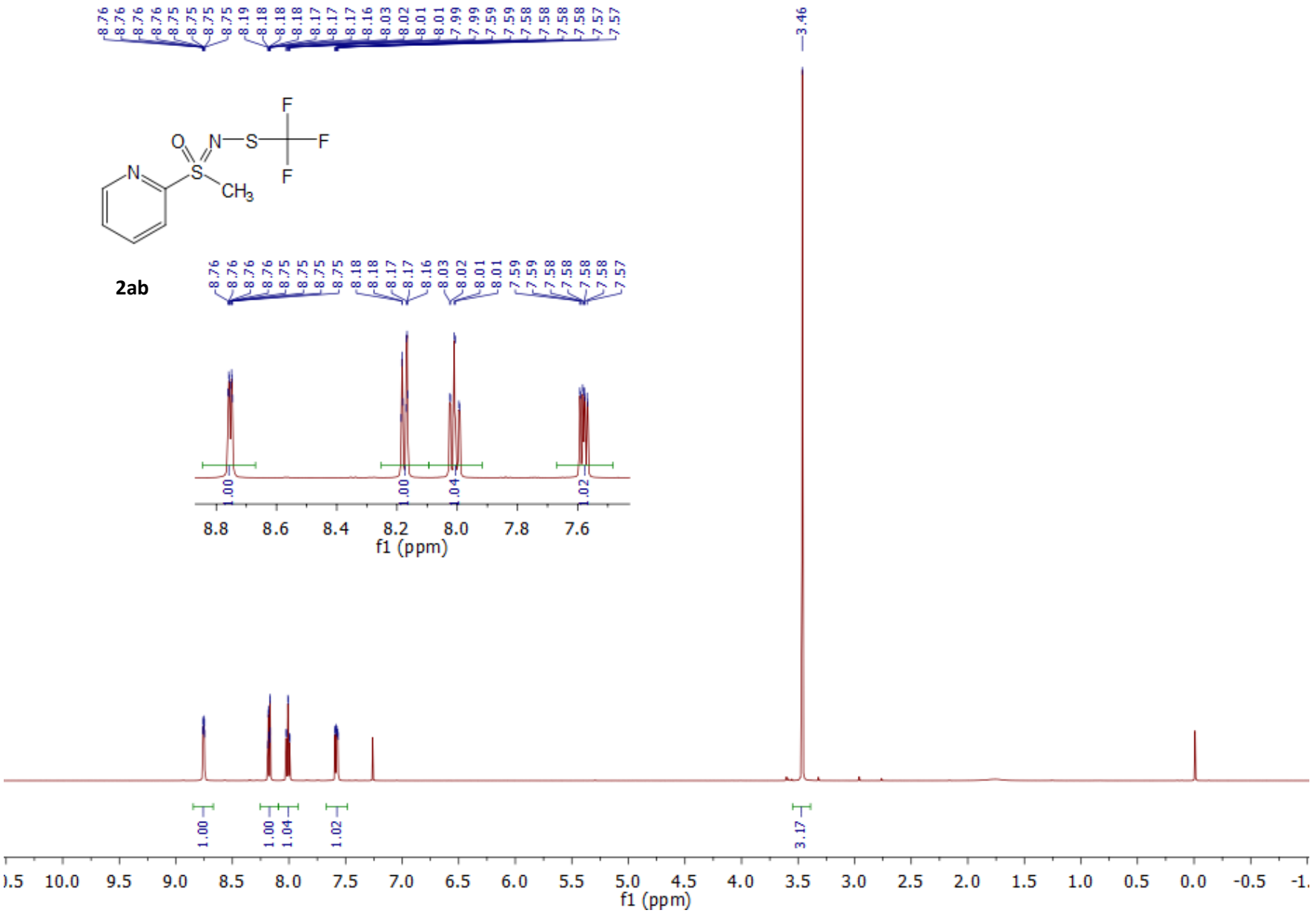
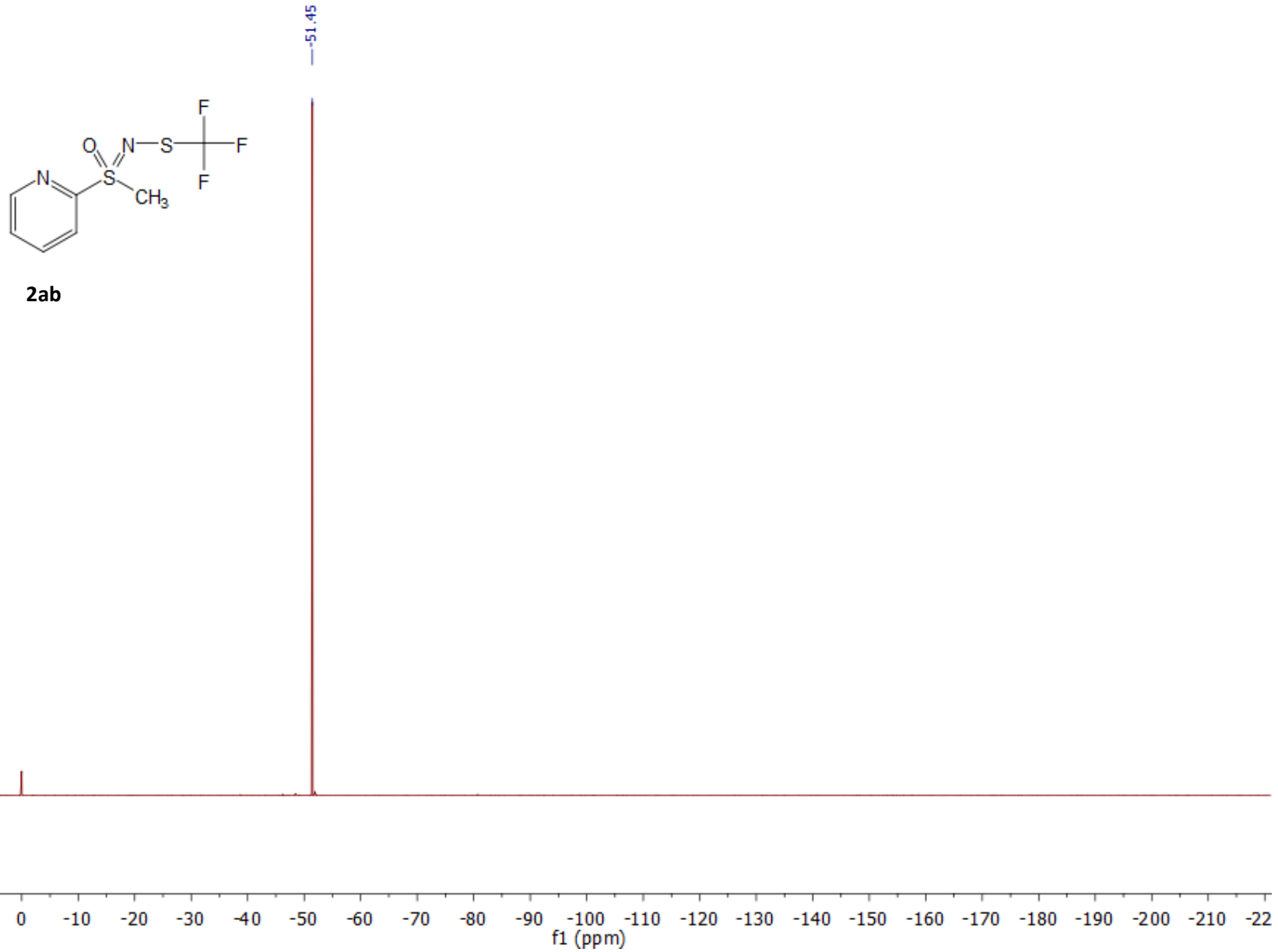
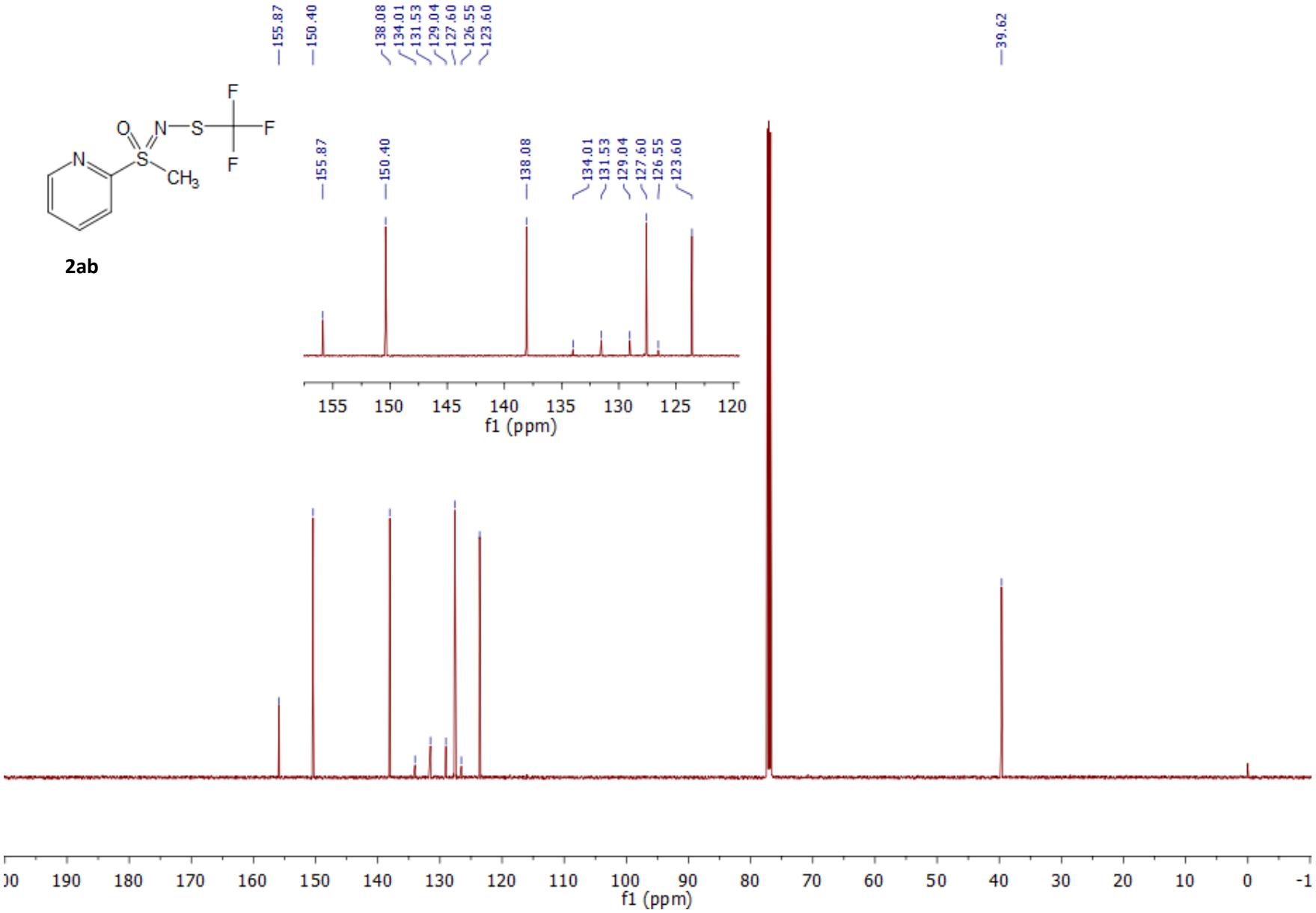
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


135.88
134.48
134.12
133.68
132.77
131.64
131.04
129.87
129.15
126.67
125.81
123.59
O
N
S
S
F
F
F
2aa
135.88
134.48
134.12
133.68
132.77
131.64
131.04
129.87
129.15
126.67
125.81
123.59
135 134 133 132 131 130 129 128 127 126
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

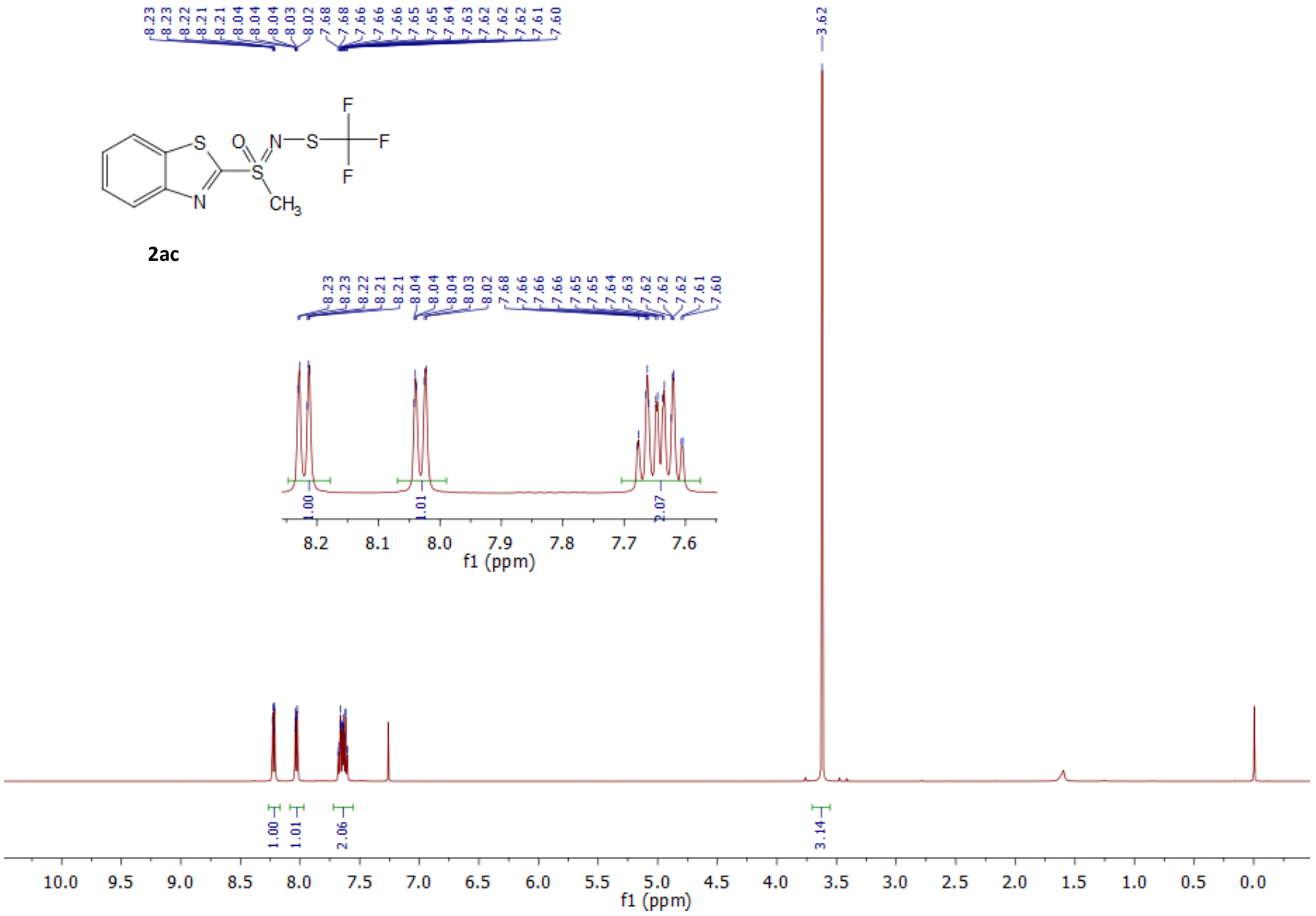

2ab
f1 (ppm)
f1 (ppm)


-51.45
F
O
N
S
F
N
S
F
CH3
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

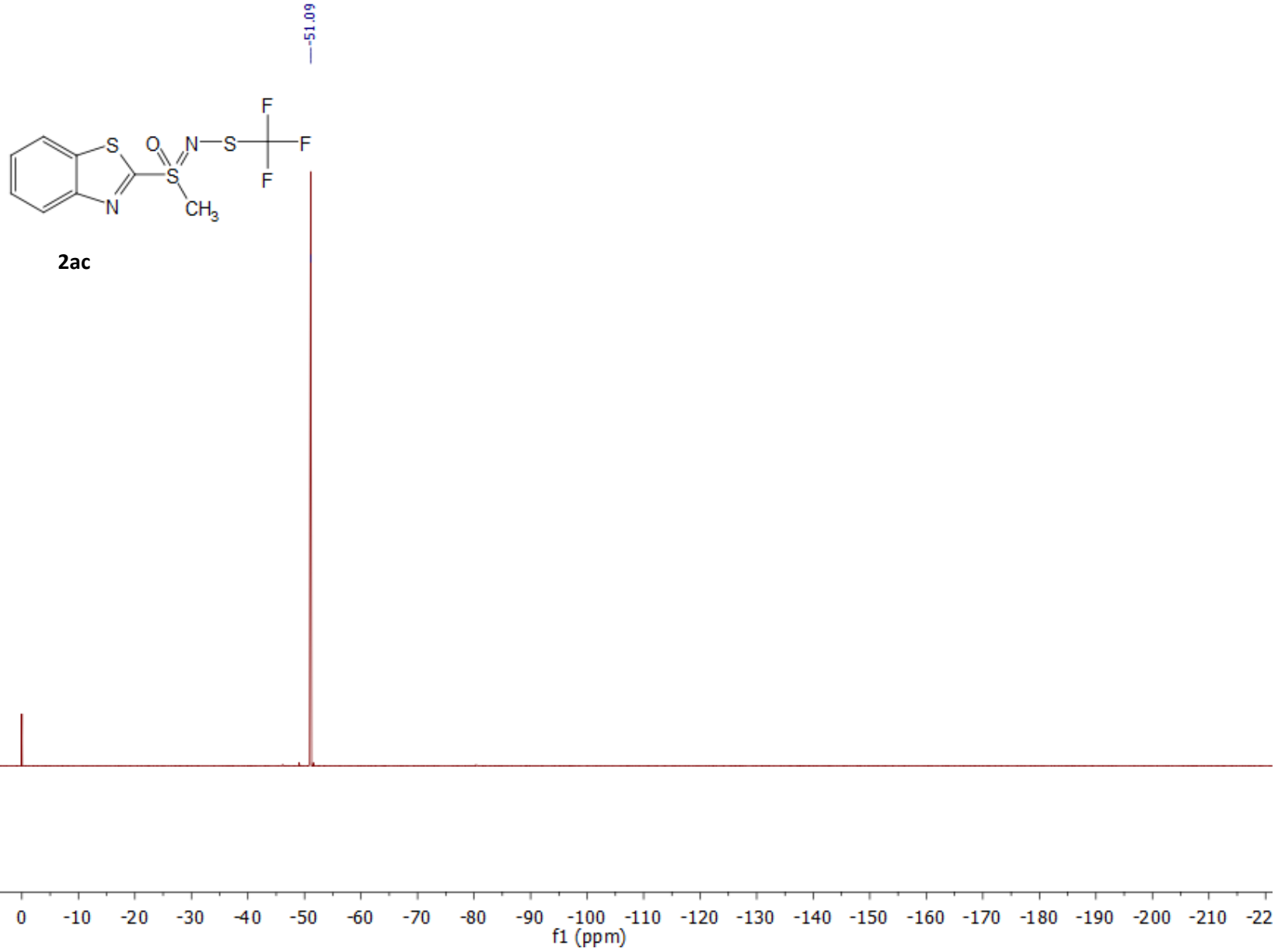
2ab


155.87
150.40
138.08
134.01
131.53
129.04
127.60
126.55
123.60
39.62
F
O
N
S
F
N
S
CH3
F
155
150
145
140
135
130
125
120
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

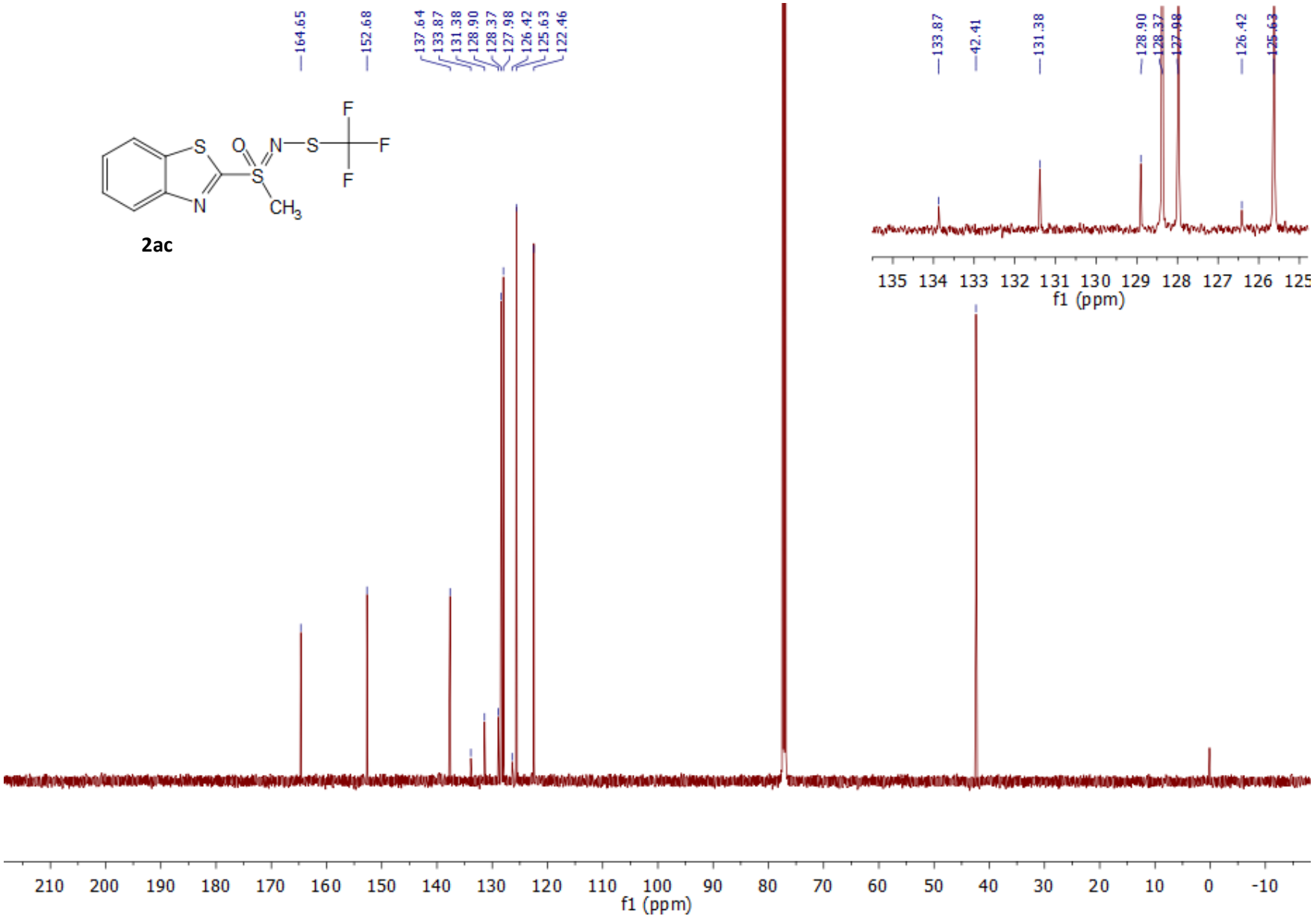
2ab

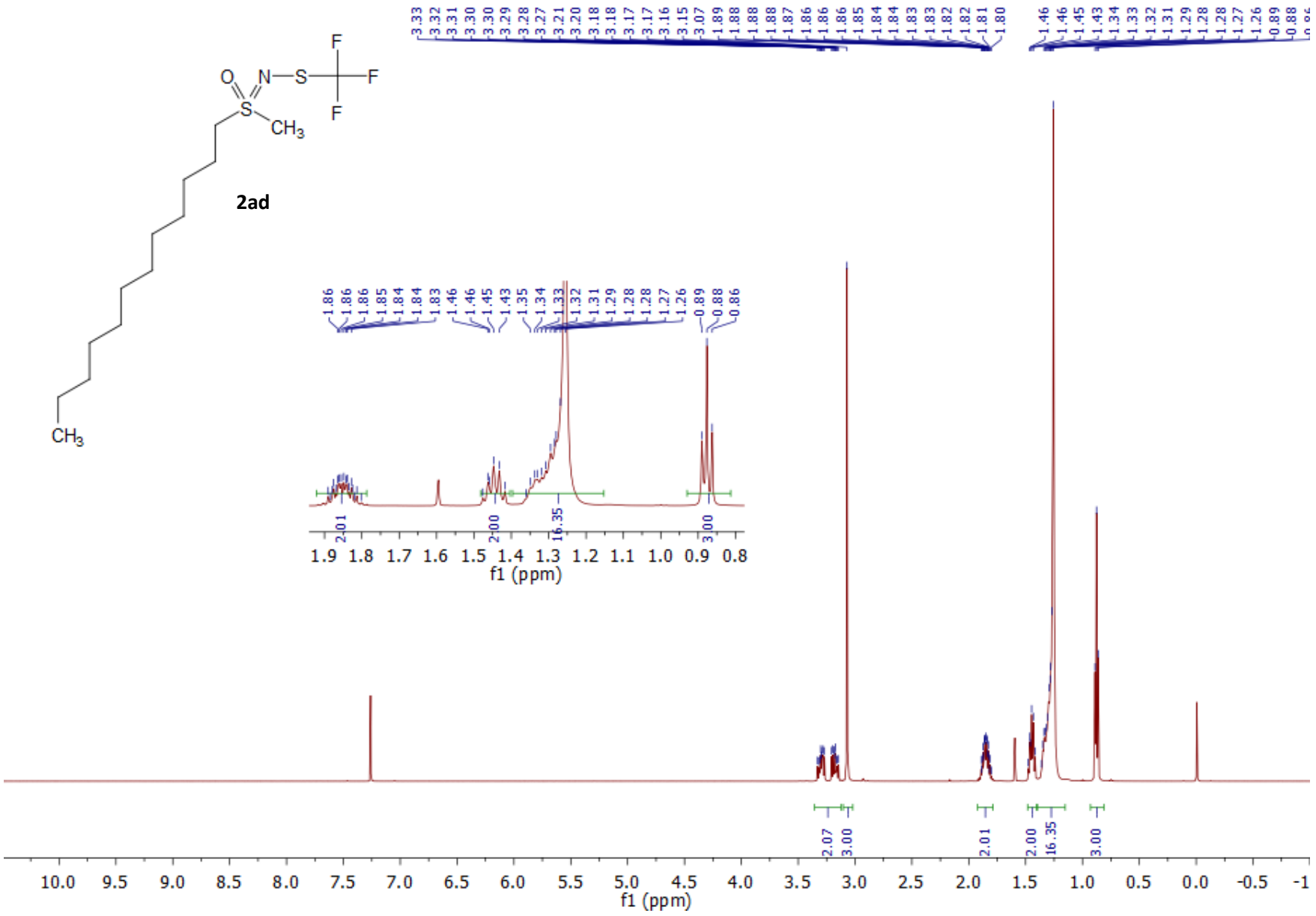

8.23
8.23
8.22
8.21
8.21
8.04
8.04
8.04
8.03
8.02
7.68
7.66
7.66
7.66
7.65
7.65
7.64
7.63
7.62
7.62
7.62
7.61
7.60
3.62
F
F
F
S
O
N
S
S
N
CH3
1.00
1.01
2.07
8.2
8.1
8.0
7.9
7.8
7.7
7.6
f1 (ppm)
1.00
1.01
2.06
3.14
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

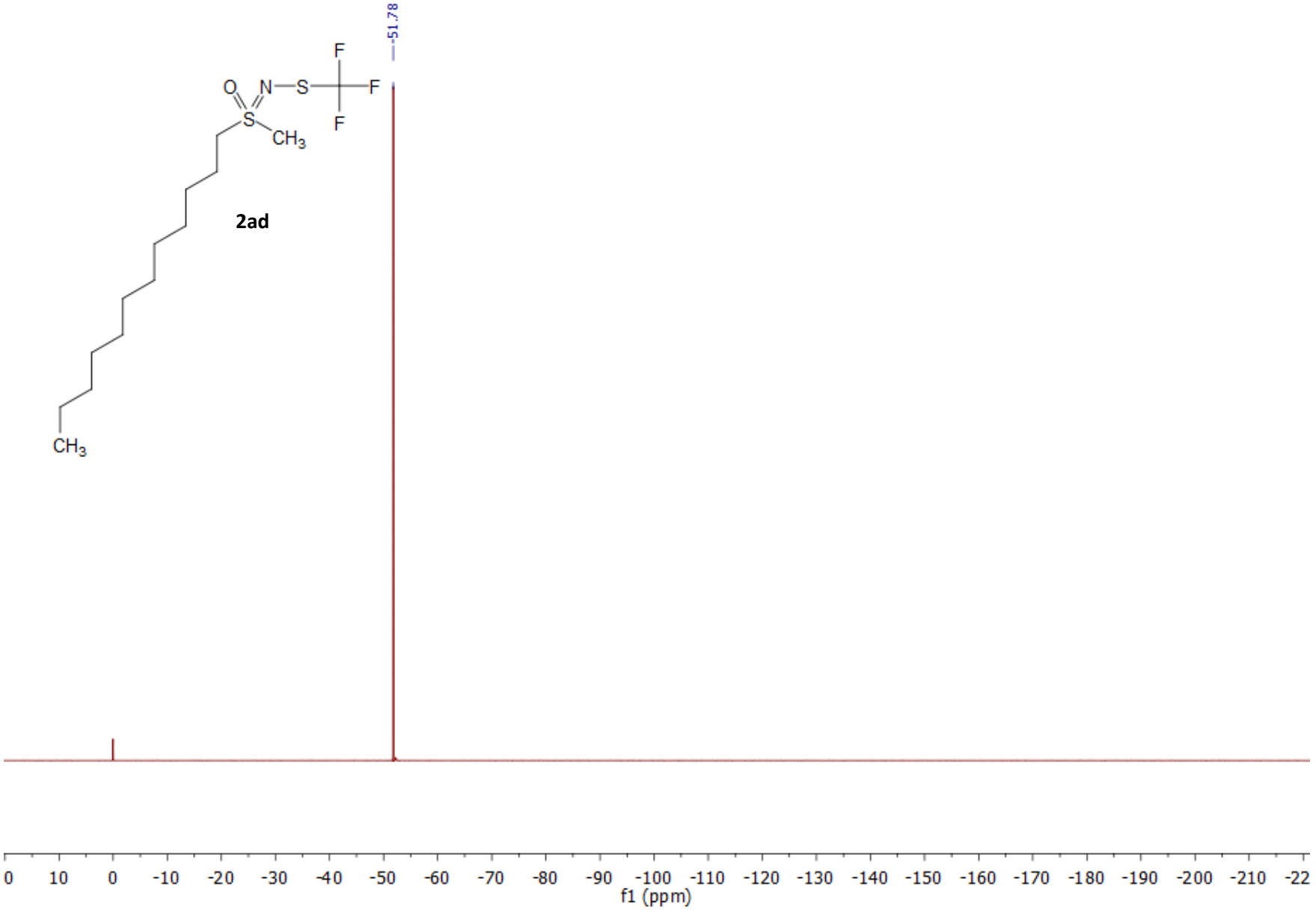
2ac

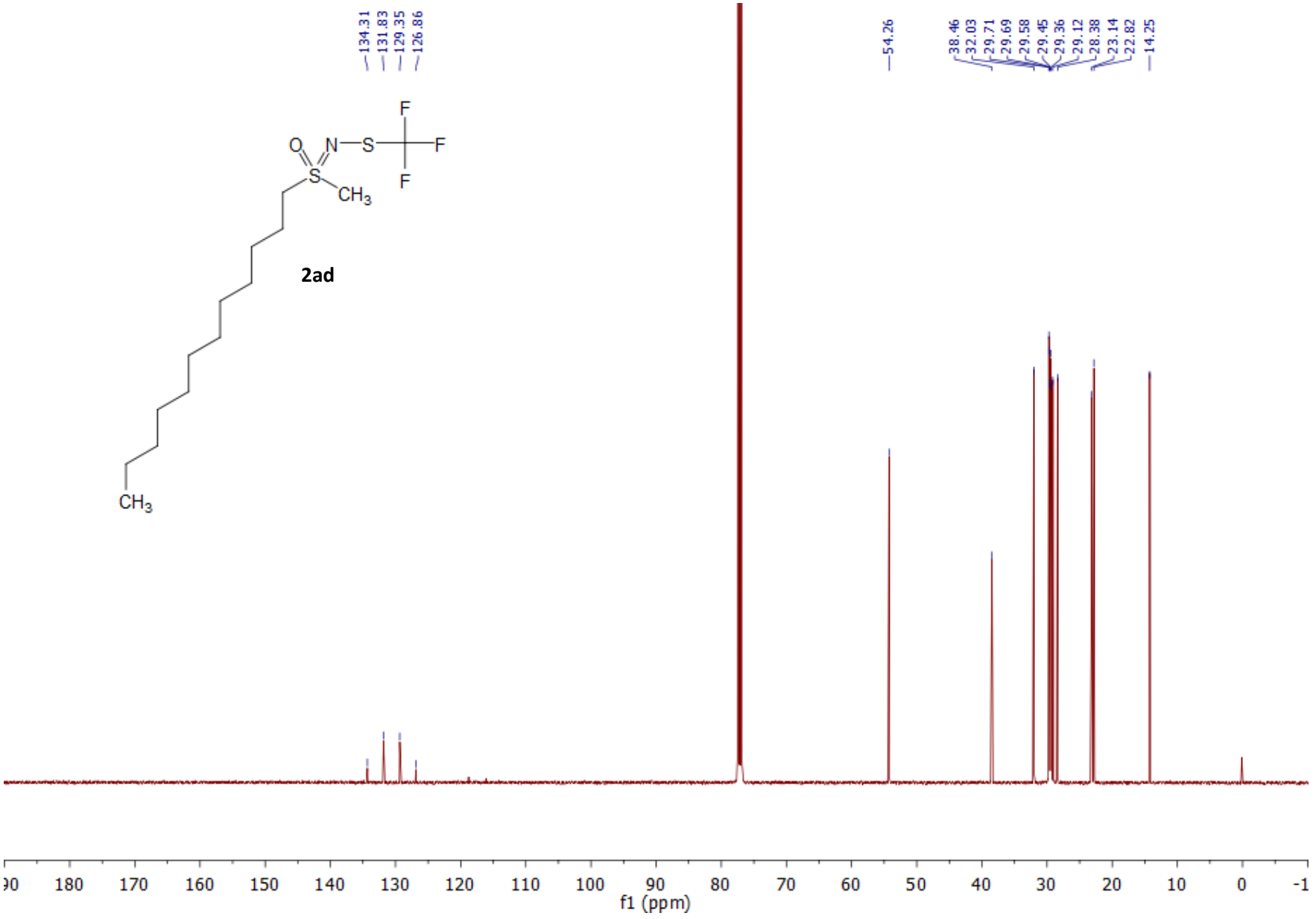

-51.09
F
S
O
N
S
F
S
F
N
CH3
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

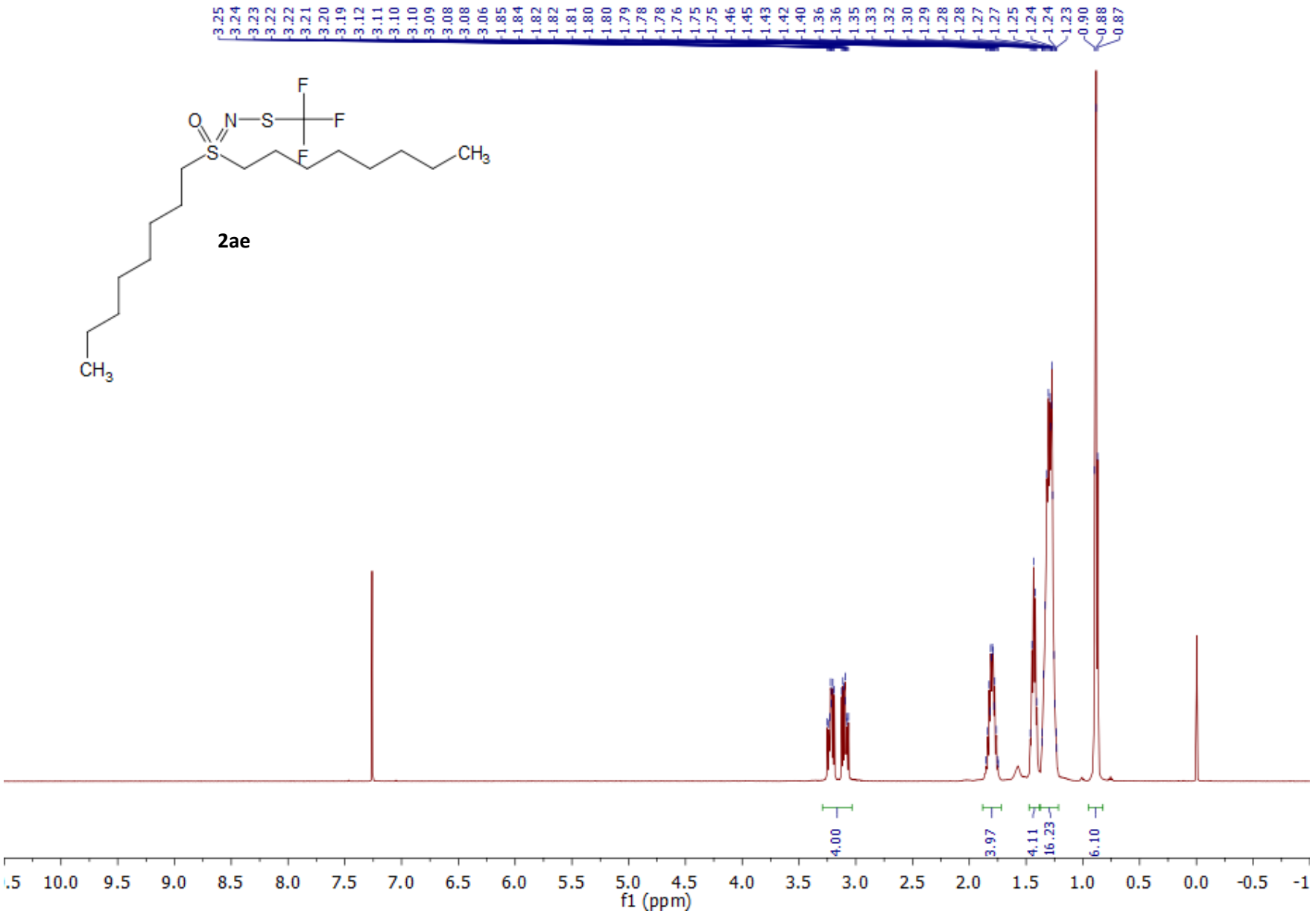
2ac

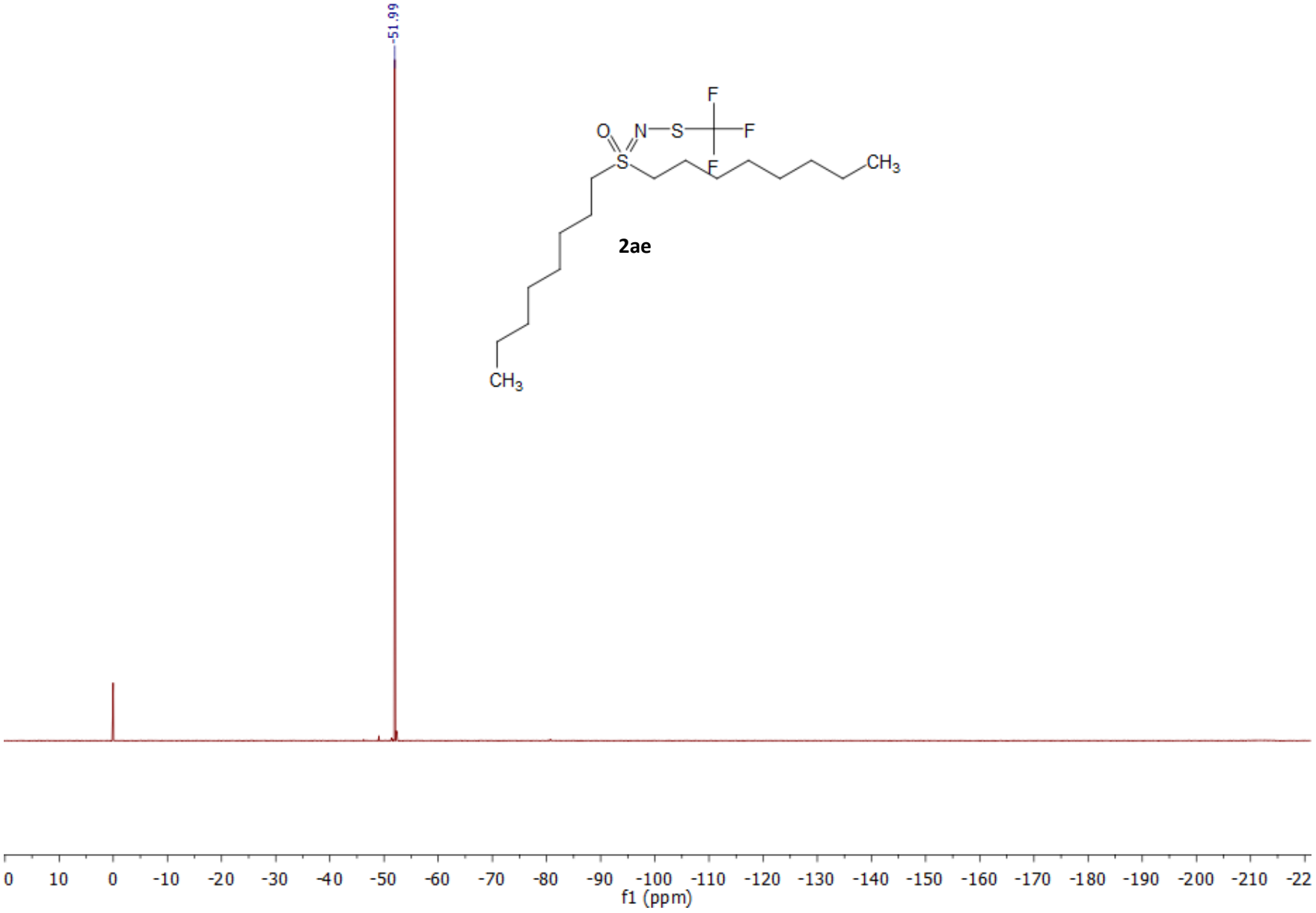

164.65
152.68
137.64
133.87
131.38
128.90
128.37
127.98
126.42
125.63
122.46
F
S
O
N
S
F
S
F
N
CH3
2ac
133.87
42.41
131.38
128.90
128.37
127.98
126.42
125.63
135 134 133 132 131 130 129 128 127 126 125
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


F
O
N
S
F
S
F
CH3
CH3
2ad
3.33 3.32 3.31 3.30 3.30 3.29 3.28 3.27 3.21 3.20 3.18 3.18 3.17 3.17 3.16 3.15 3.07 1.89 1.88 1.88 1.87 1.86 1.86 1.86 1.85 1.84 1.84 1.83 1.83 1.82 1.82 1.81 1.80
1.46 1.46 1.45 1.43 1.34 1.33 1.32 1.31 1.29 1.28 1.28 1.27 1.26 0.89 0.88
1.86 1.86 1.86 1.85 1.84 1.84 1.83 1.46 1.46 1.45 1.43 1.35 1.34 1.33 1.32 1.31 1.29 1.28 1.28 1.27 1.26 0.89 0.88 0.86
2.01 2.00 16.35 3.00
1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8
f1 (ppm)
2.07 3.00 2.01 2.00 16.35 3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

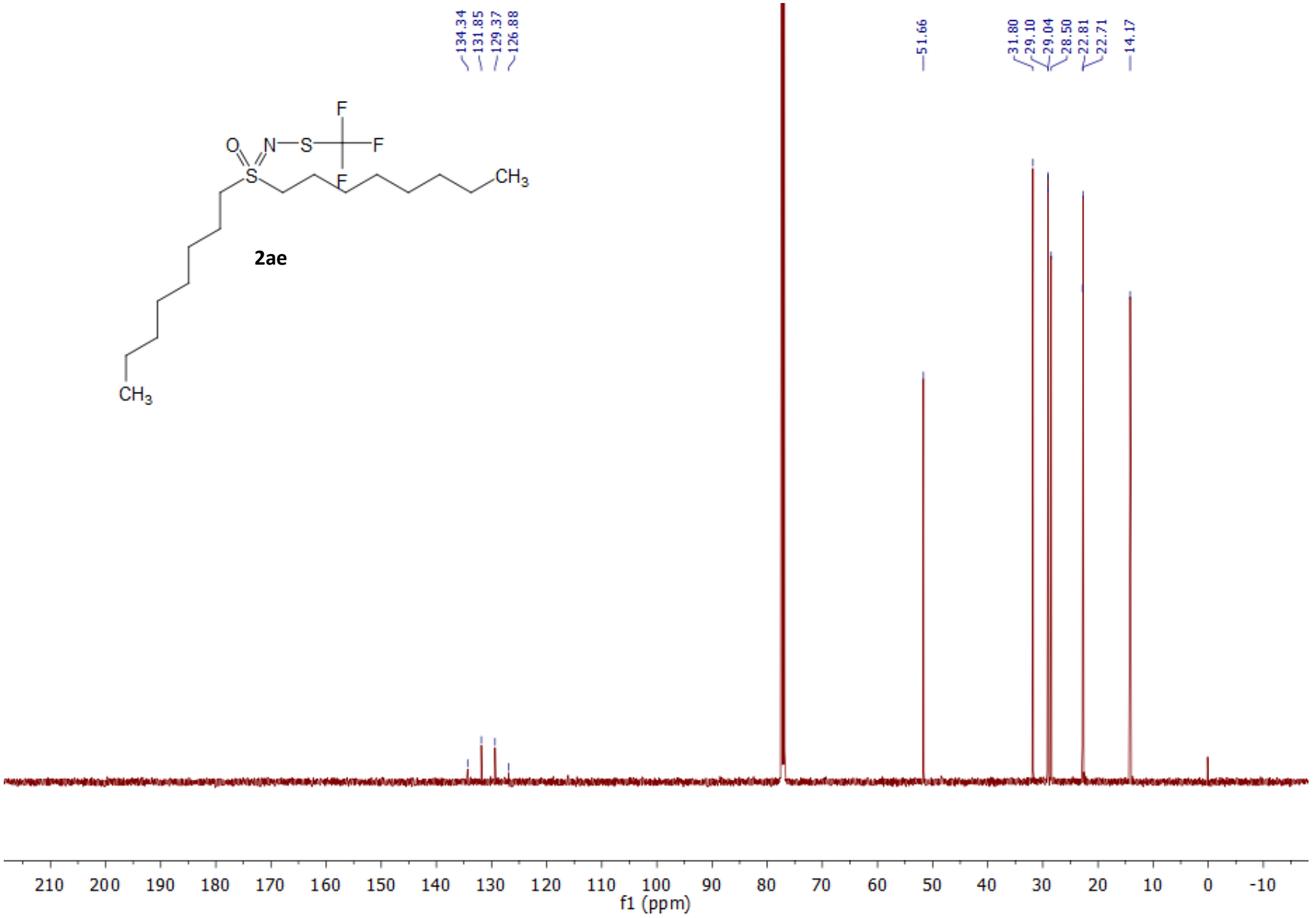

-51.78
F
O
N
S
F
S
F
CH3
CH3
2ad
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

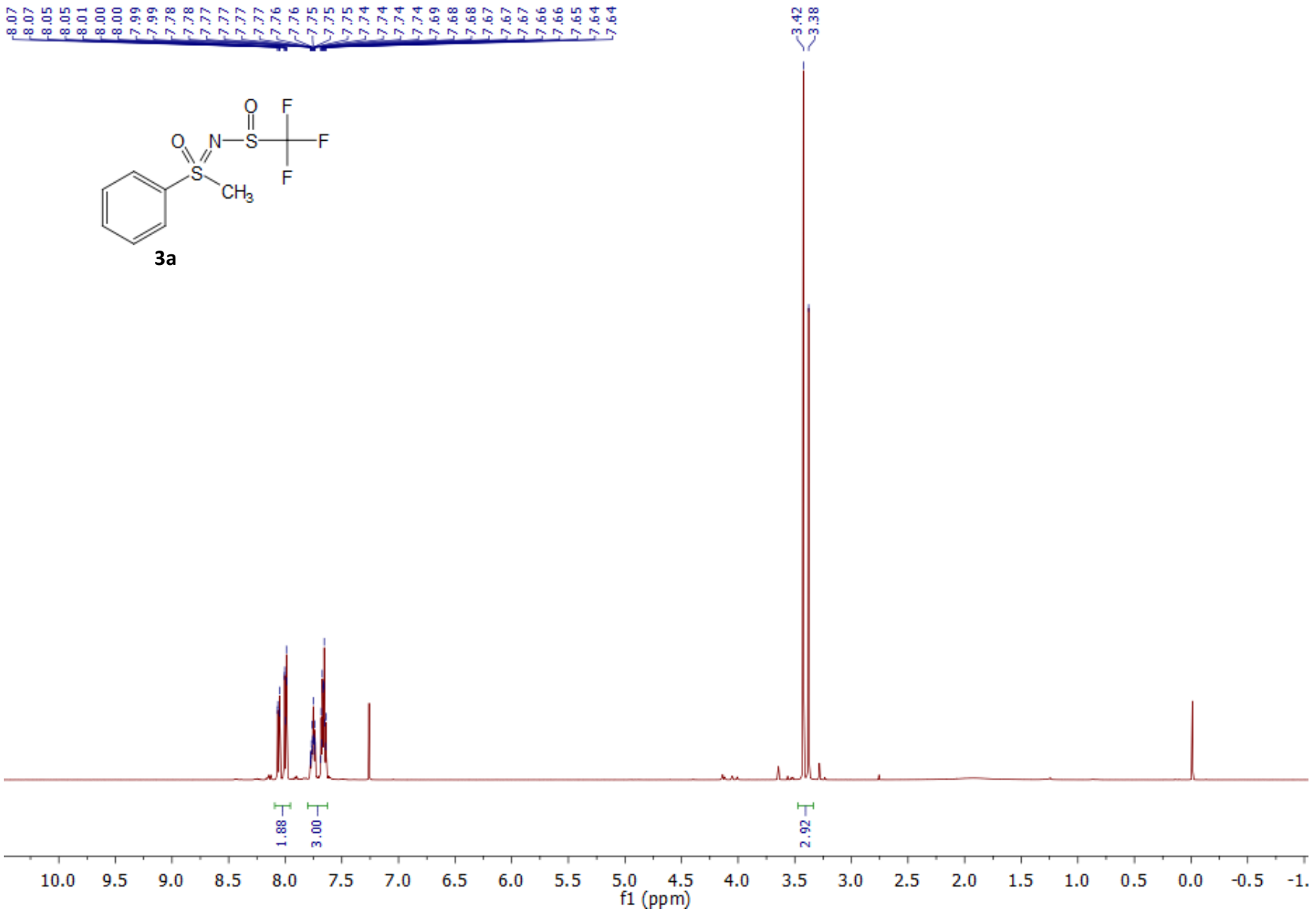

134.31
131.83
129.35
126.86
54.26
38.46
32.03
29.71
29.69
29.58
29.45
29.36
29.12
28.38
23.14
22.82
14.25
O
N
S
F
F
F
S
CH3
CH3
2ad
f1 (ppm)


3.25 3.24 3.23 3.22 3.22 3.21 3.20 3.19 3.12 3.11 3.10 3.10 3.09 3.08 3.08 3.06 1.85 1.84 1.82 1.82 1.81 1.80 1.80 1.79 1.78 1.78 1.76 1.75 1.75 1.46 1.45 1.43 1.42 1.40 1.36 1.36 1.35 1.33 1.32 1.30 1.29 1.28 1.28 1.27 1.27 1.25 1.24 1.24 1.23 0.90 0.88 0.87
O
N
S
F
F
F
S
CH3
CH3
2ae
4.00
3.97
4.11
16.23
6.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


-51.99
F
O
N
S
F
S
F
CH3
CH3
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

2ae

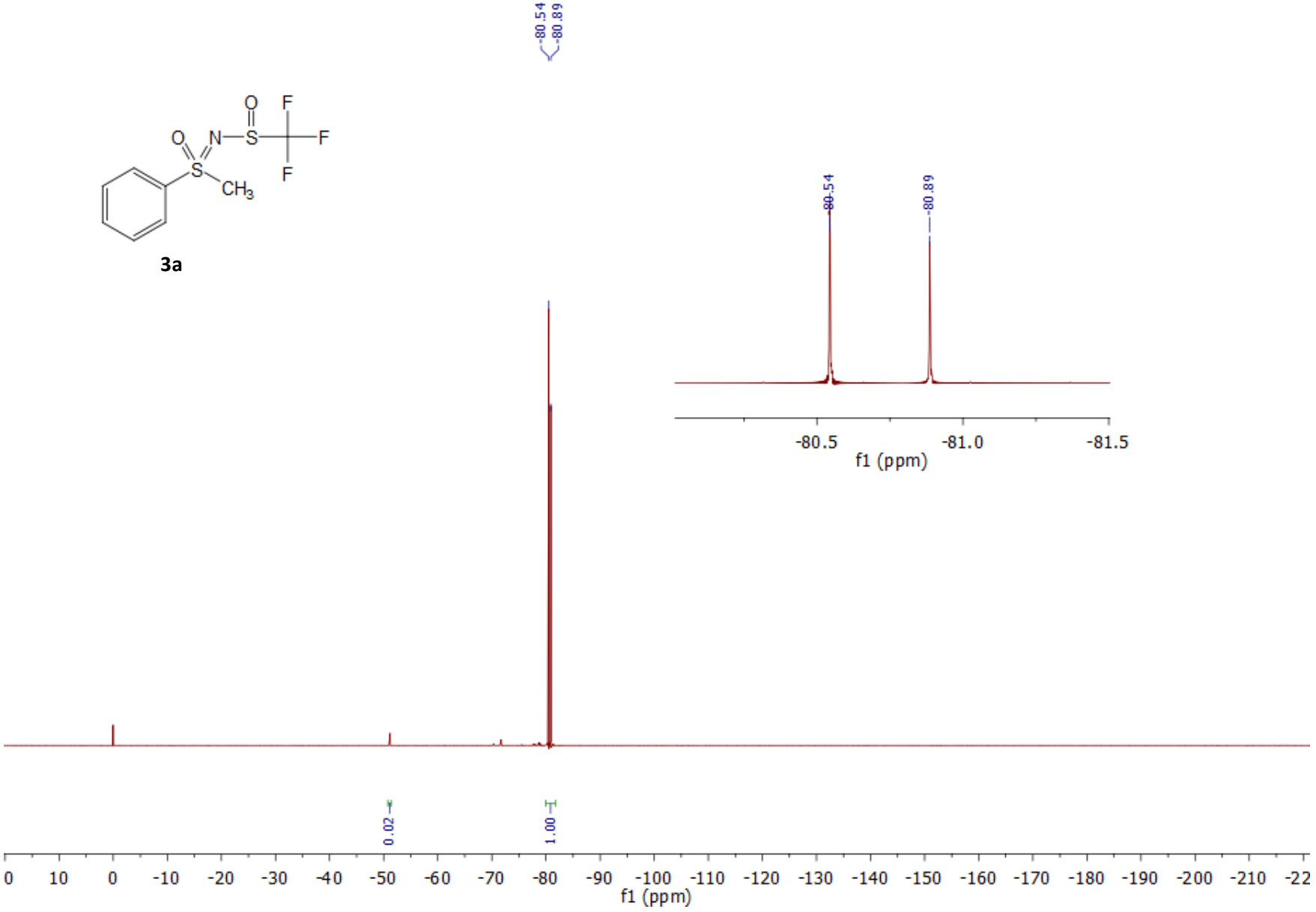

134.34
131.85
129.37
126.88
51.66
31.80
29.10
29.04
28.50
22.81
22.71
14.17
F
O
N
S
F
S
F
CH3
CH3
2ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

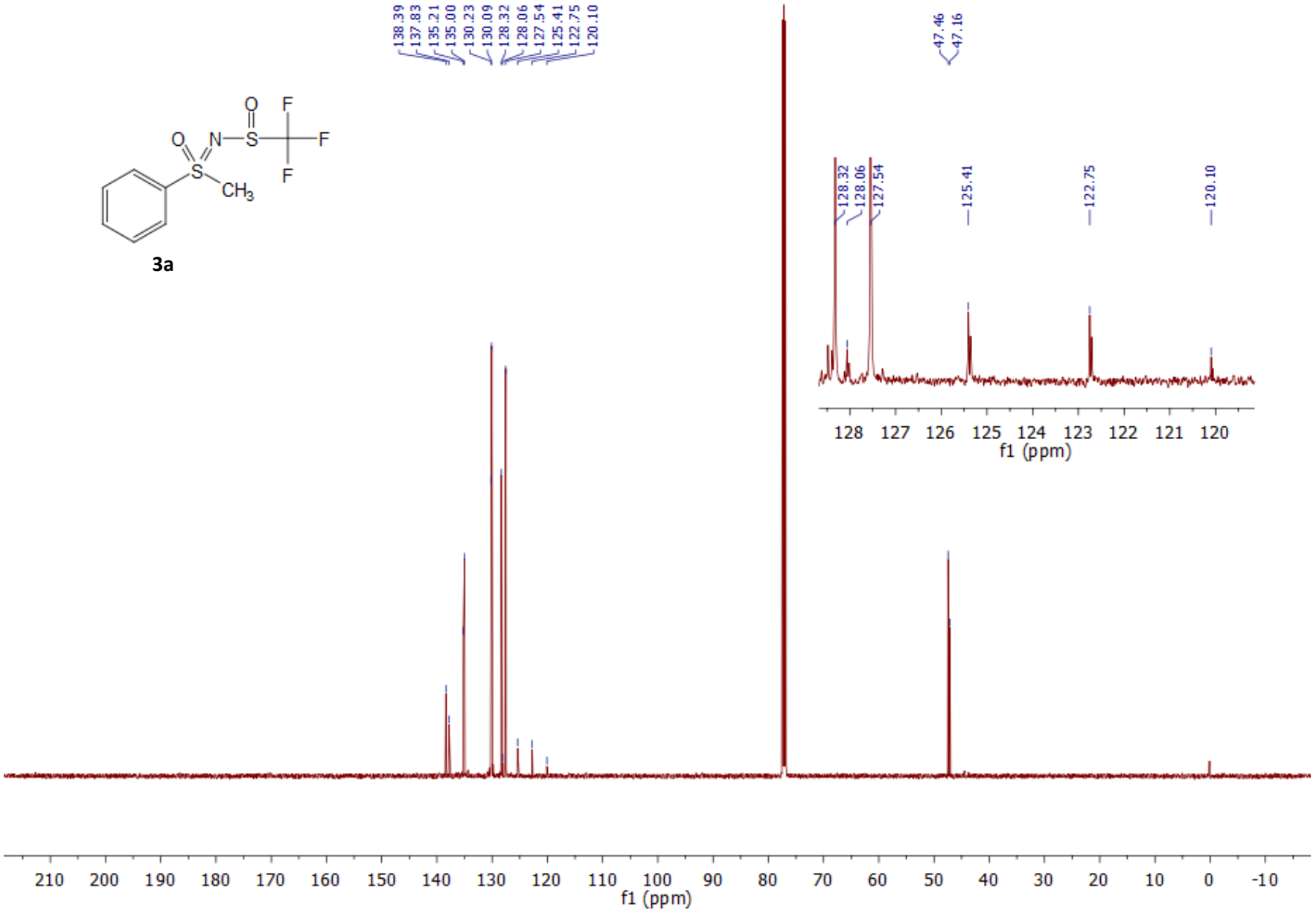

8.07
8.07
8.05
8.05
8.01
8.00
8.00
7.99
7.99
7.78
7.78
7.77
7.77
7.77
7.77
7.76
7.76
7.75
7.75
7.75
7.74
7.74
7.74
7.74
7.69
7.68
7.68
7.67
7.67
7.67
7.66
7.66
7.65
7.64
7.64
3.42
3.38
O
F
O
N
S
F
S
F
CH3
1.88
3.00
2.92
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)

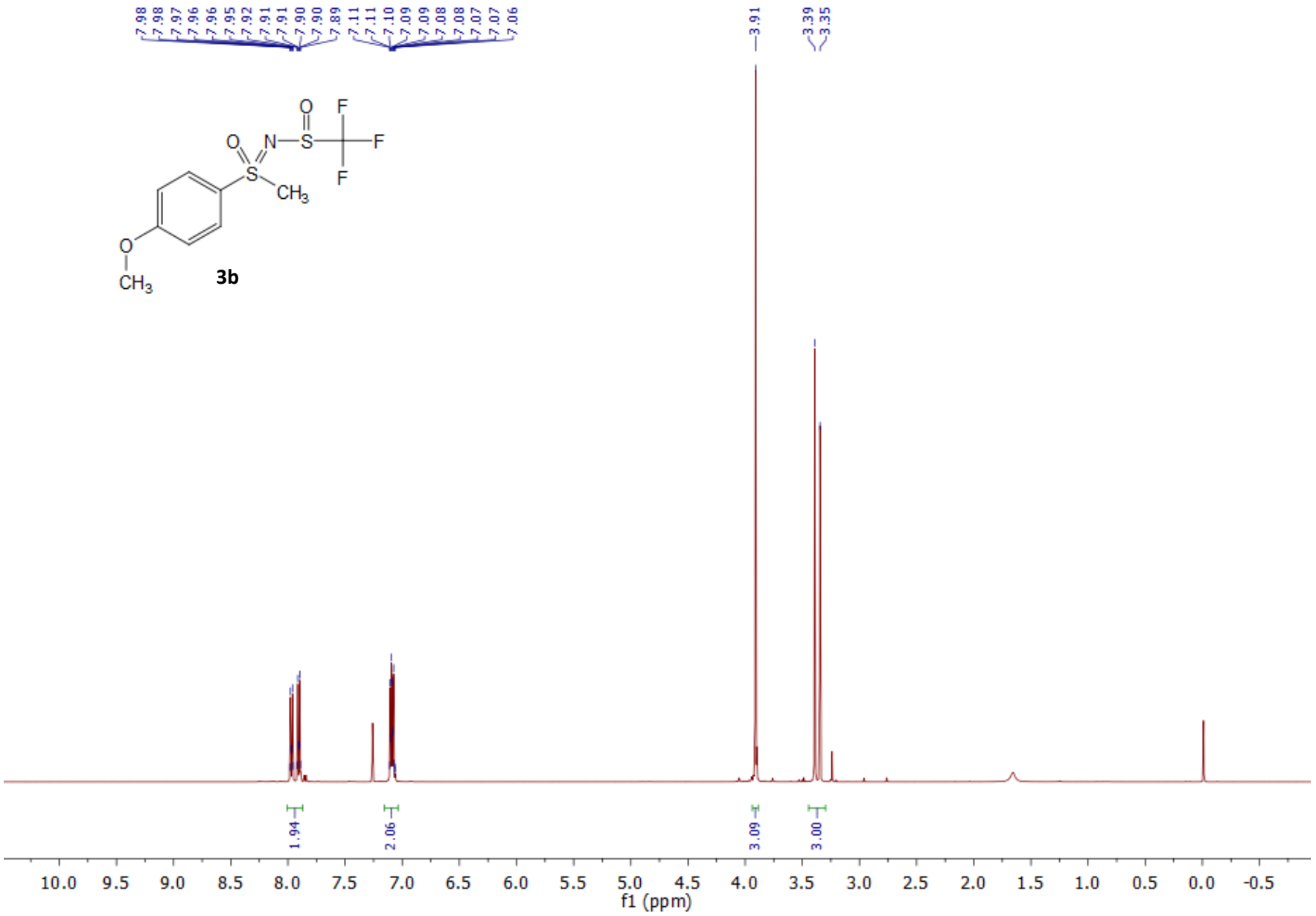
3a

O
F
O
N
S
F
S
F
CH3

3a


-80.54
-80.89
-80.54
-80.89
-80.5
-81.0
-81.5
f1 (ppm)
0.02
1.00
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


138.39
137.83
135.21
135.00
130.23
130.09
128.32
128.06
127.54
125.41
122.75
120.10
47.46
47.16
O
F
O
N
S
F
S
F
CH3
3a
128.32
128.06
127.54
125.41
122.75
120.10
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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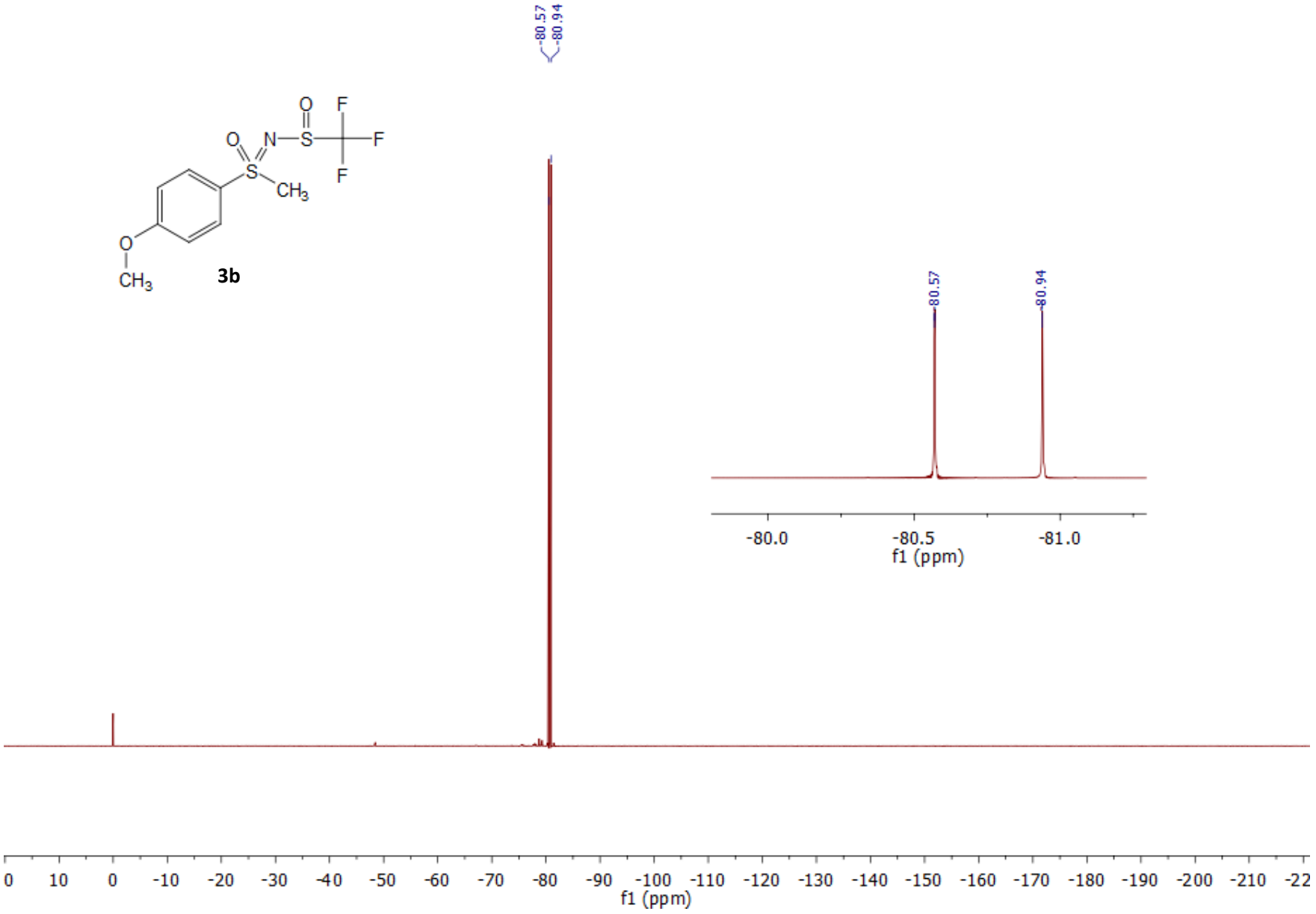
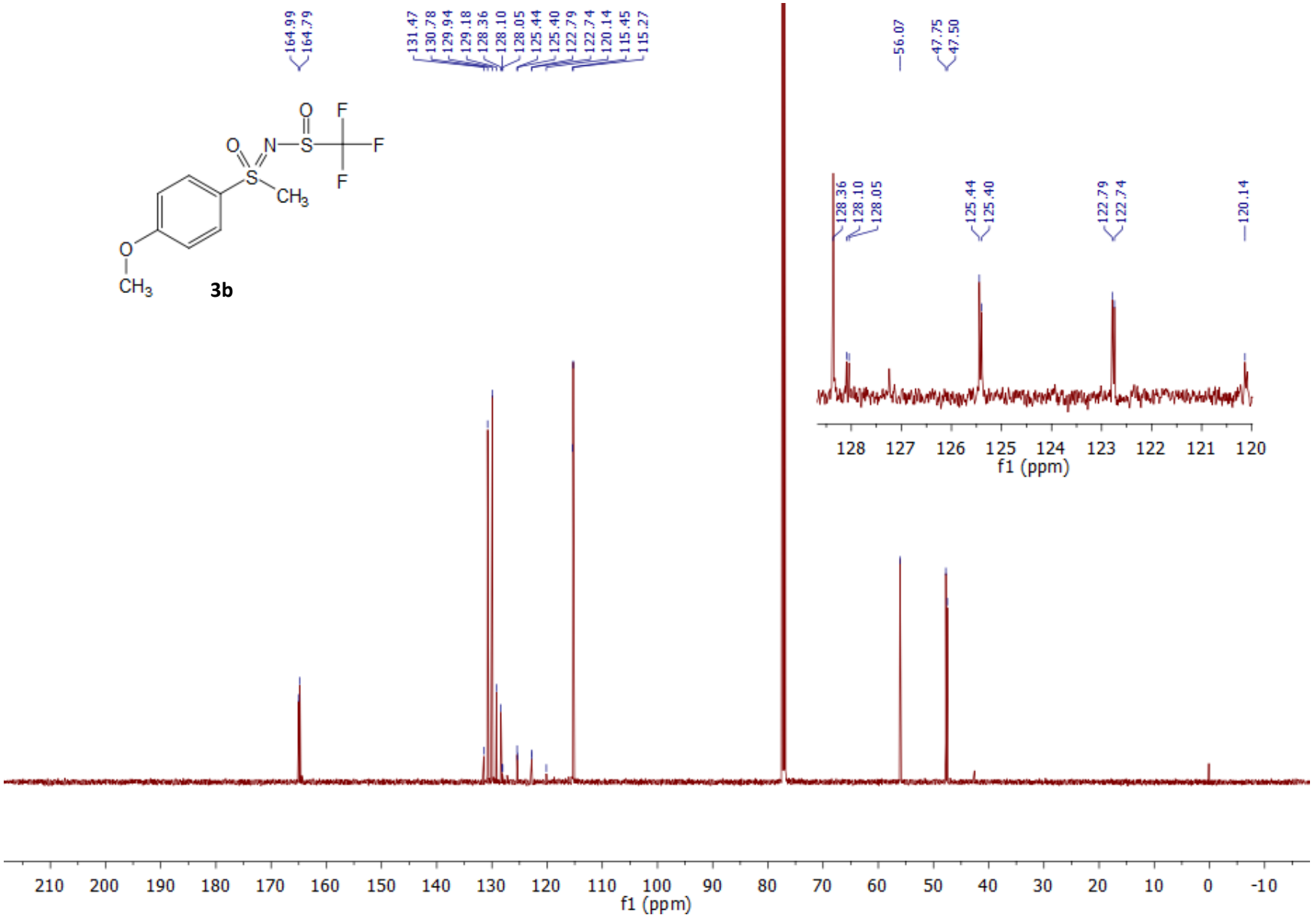
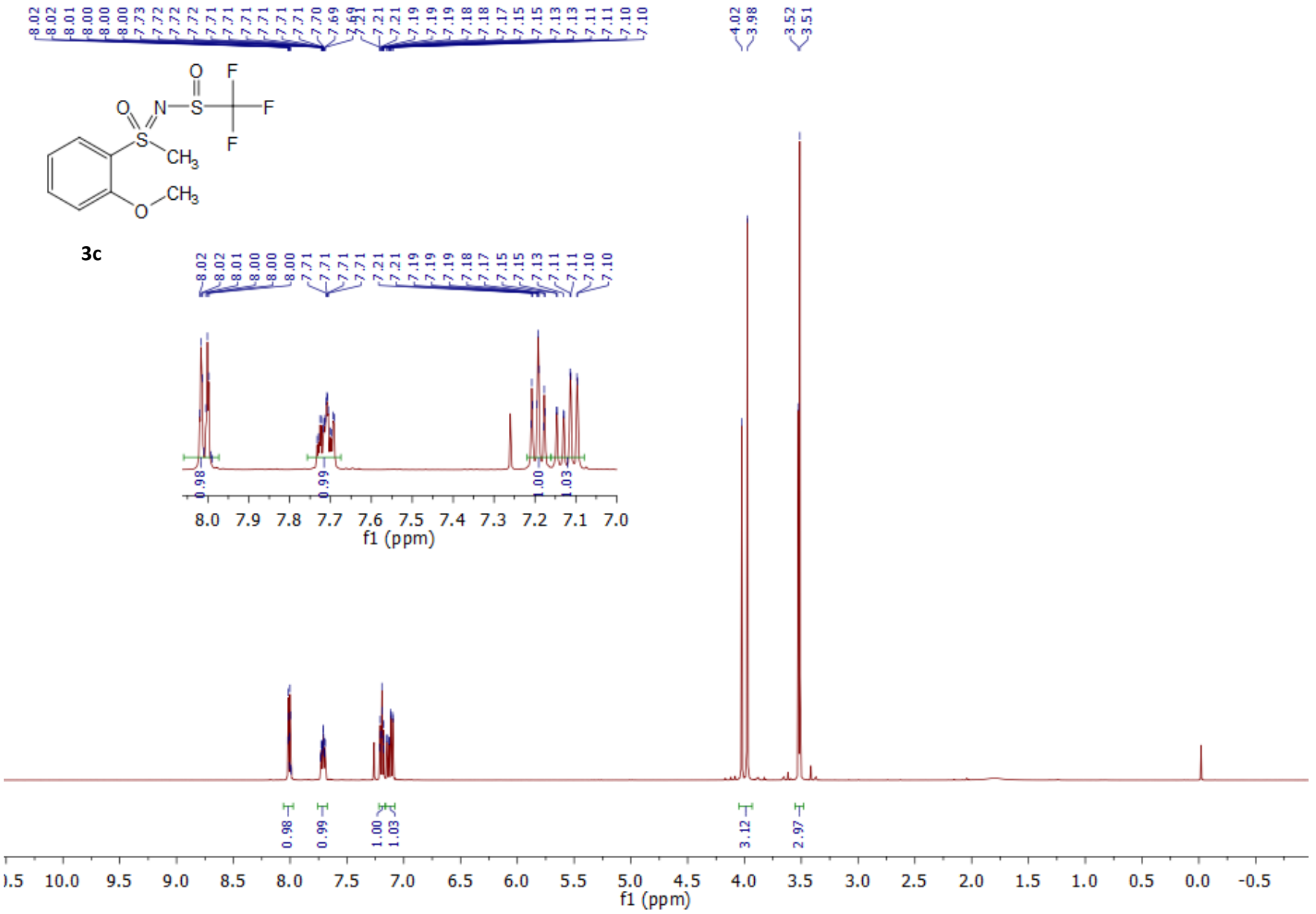
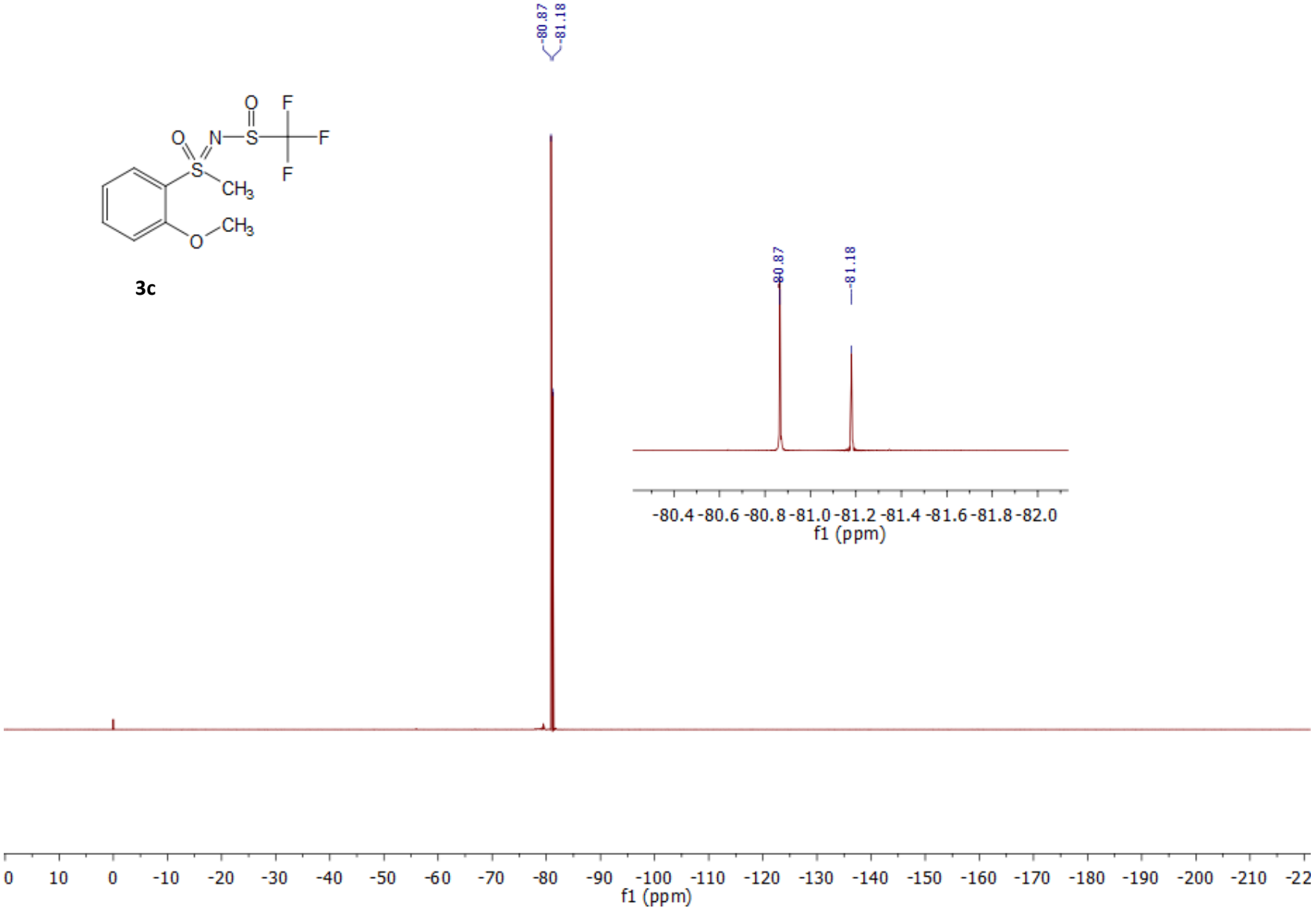
7.98
7.97
7.96
7.96
7.95
7.92
7.91
7.91
7.90
7.90
7.89
7.11
7.11
7.10
7.09
7.09
7.08
7.08
7.07
7.07
7.06
3.91
3.39
3.35
O
F
O
N
S
F
S
CH3
F
O
CH3
1.94
2.06
3.09
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

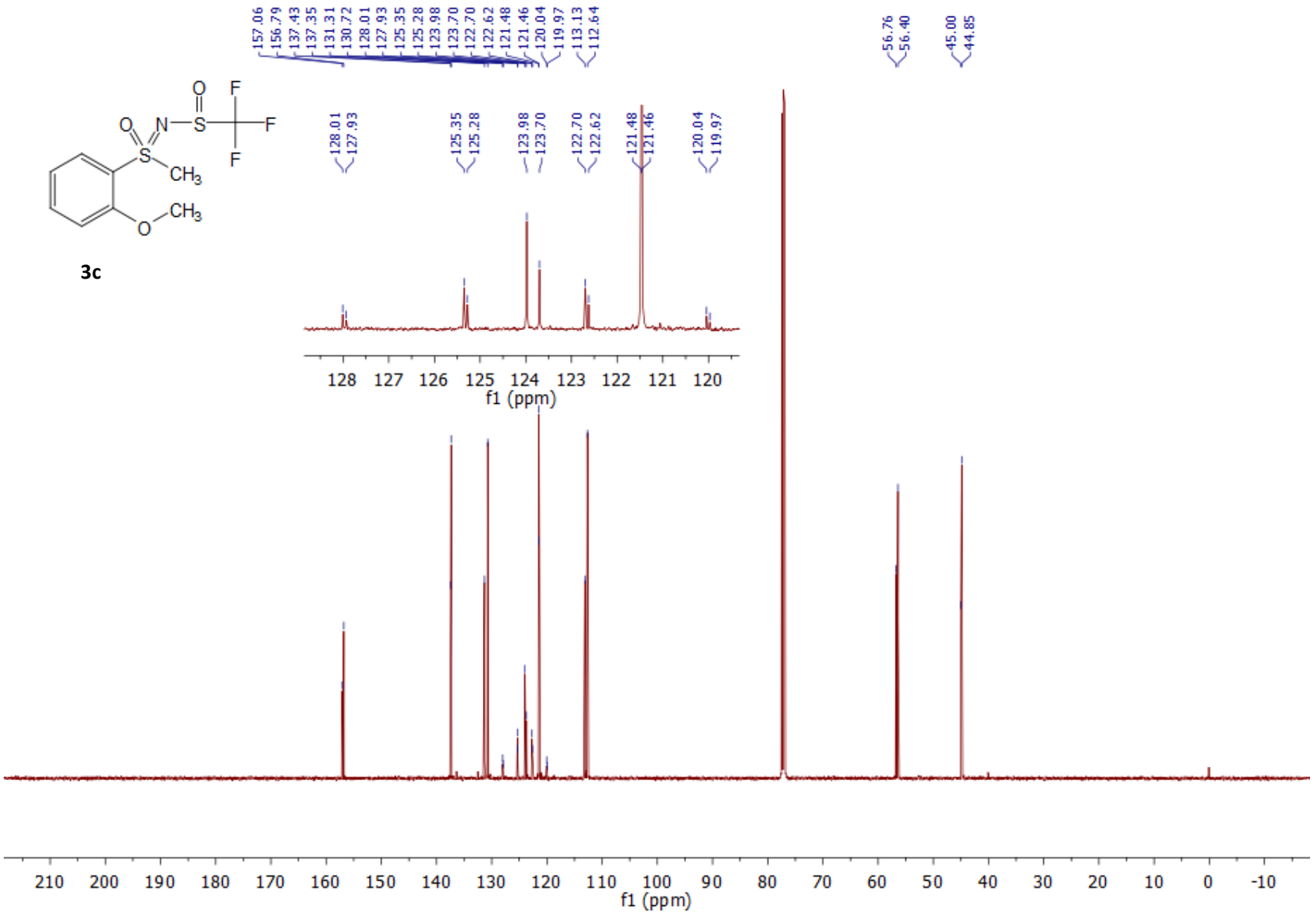
3b

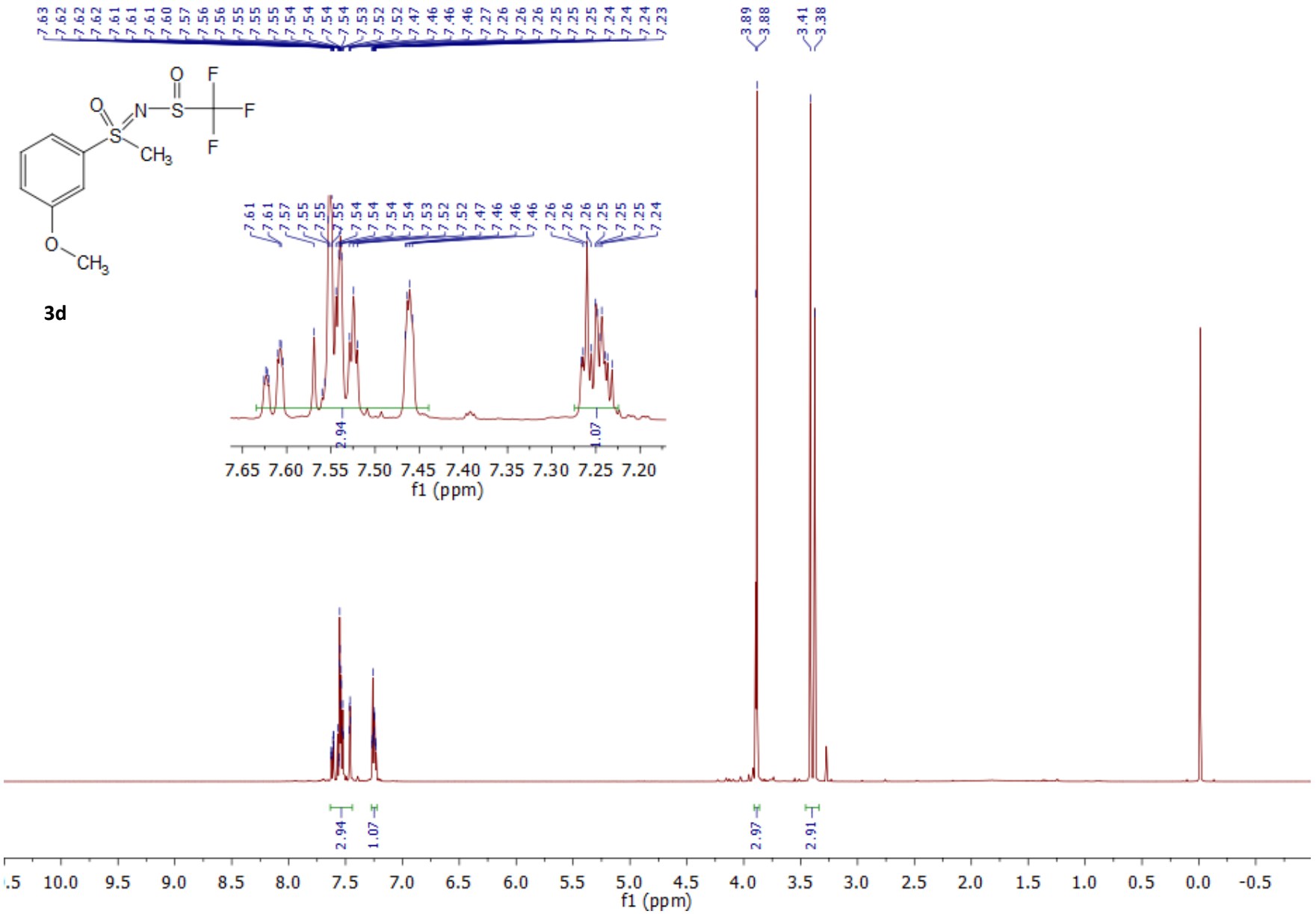

-80.57
-80.94
O
F
O
N
S
F
S
F
CH3
O
CH3
3b
80.57
80.94
-80.0
-80.5
-81.0
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

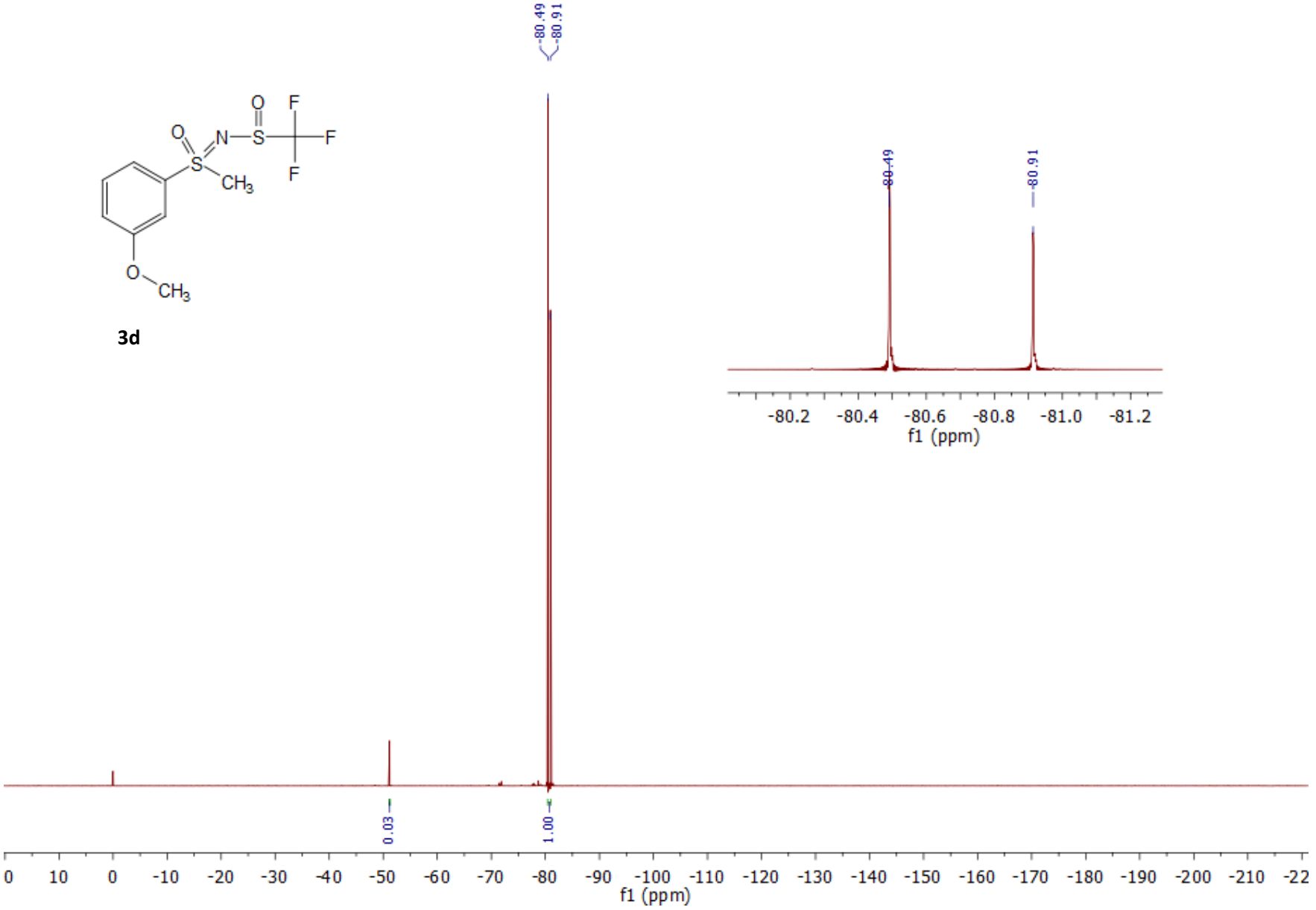

164.99
164.79
131.47
130.78
129.94
129.18
128.36
128.10
128.05
125.44
125.40
122.79
122.74
120.14
115.45
115.27
56.07
47.75
47.50
O
F
O
N
S
F
S
F
CH3
O
CH3
3b
128.36
128.10
128.05
125.44
125.40
122.79
122.74
120.14
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.02 8.02 8.01 8.00 8.00 8.00 7.73 7.72 7.72 7.72 7.71 7.71 7.71 7.71 7.71 7.71 7.70 7.69 7.69 7.21 7.21 7.19 7.19 7.19 7.18 7.18 7.17 7.15 7.15 7.13 7.11 7.11 7.10 7.10
4.02 3.98 3.52 3.51
O F O N S F F CH3 CH3 O
3c
8.02 8.02 8.01 8.00 8.00 8.00 7.71 7.71 7.71 7.71 7.21 7.21 7.19 7.19 7.19 7.18 7.17 7.15 7.15 7.13 7.11 7.11 7.10 7.10
0.98 0.99 1.00 1.03
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
0.98 0.99 1.00 1.03 3.12 2.97
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

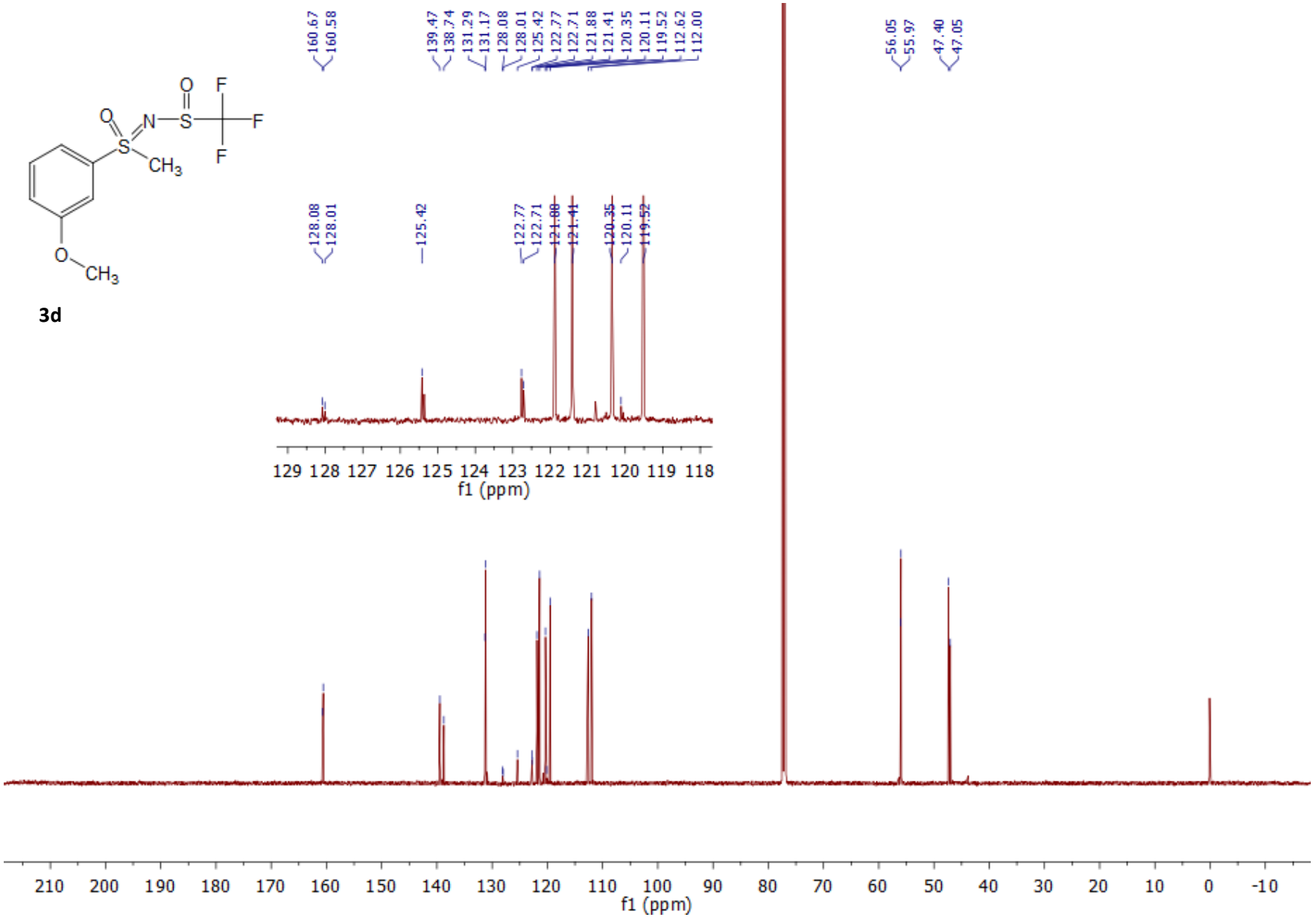

-80.87
-81.18
O
F
O
N
S
F
S
F
CH3
CH3
O
3c
-80.87
-81.18
-80.4 -80.6 -80.8 -81.0 -81.2 -81.4 -81.6 -81.8 -82.0
f1 (ppm)
0 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)


157.06
156.79
137.43
137.35
131.31
130.72
128.01
127.93
125.35
125.28
123.98
123.70
122.70
122.62
121.48
121.46
120.04
119.97
113.13
112.64
56.76
56.40
45.00
44.85
O
F
O
N
S
F
S
F
CH3
CH3
O
3c
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

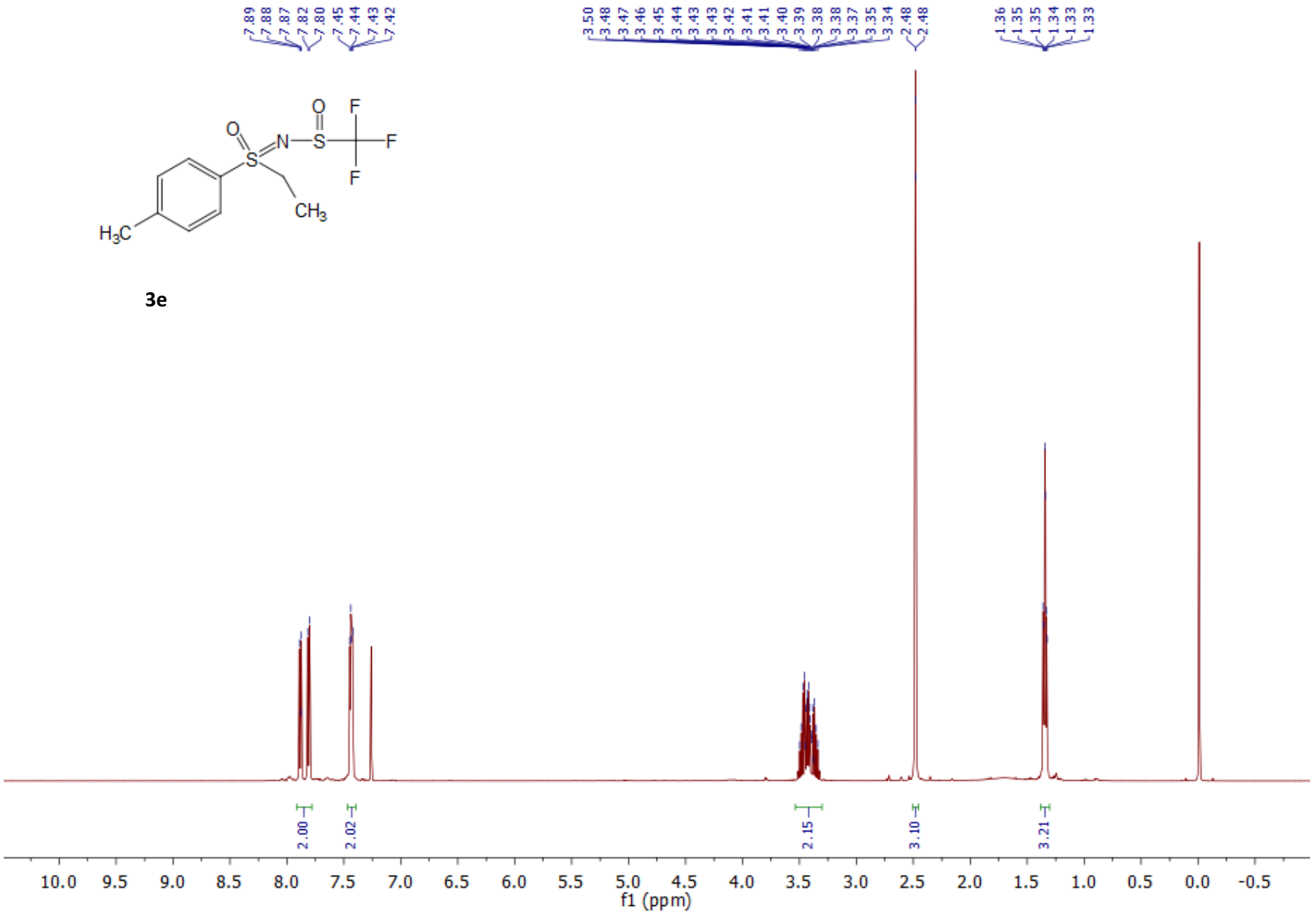

7.63 7.62 7.62 7.62 7.61 7.61 7.61 7.60 7.57 7.56 7.56 7.55 7.55 7.55 7.54 7.54 7.54 7.54 7.53 7.52 7.52 7.47 7.46 7.46 7.46 7.27 7.26 7.26 7.26 7.25 7.25 7.25 7.24 7.24 7.24 7.23
3.89 3.88 3.41 3.38
O F O N S F S F CH3 O CH3
3d
7.61 7.61 7.57 7.55 7.55 7.55 7.54 7.54 7.54 7.54 7.53 7.52 7.52 7.47 7.46 7.46 7.46 7.26 7.26 7.26 7.25 7.25 7.25 7.24
2.94 1.07
7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20
f1 (ppm)
2.94 1.07 2.97 2.91
.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


-80.49
-80.91
O
F
O
N
S
F
S
F
CH3
O
CH3
-80.49
-80.91
-80.2
-80.4
-80.6
-80.8
-81.0
-81.2
f1 (ppm)
0.03
1.00
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

3d


160.67
160.58
139.47
138.74
131.29
131.17
128.08
128.01
125.42
122.77
122.71
121.88
121.41
120.35
120.11
119.52
112.62
112.00
56.05
55.97
47.40
47.05
O
F
O
N
S
F
S
CH3
F
O
CH3
129 128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

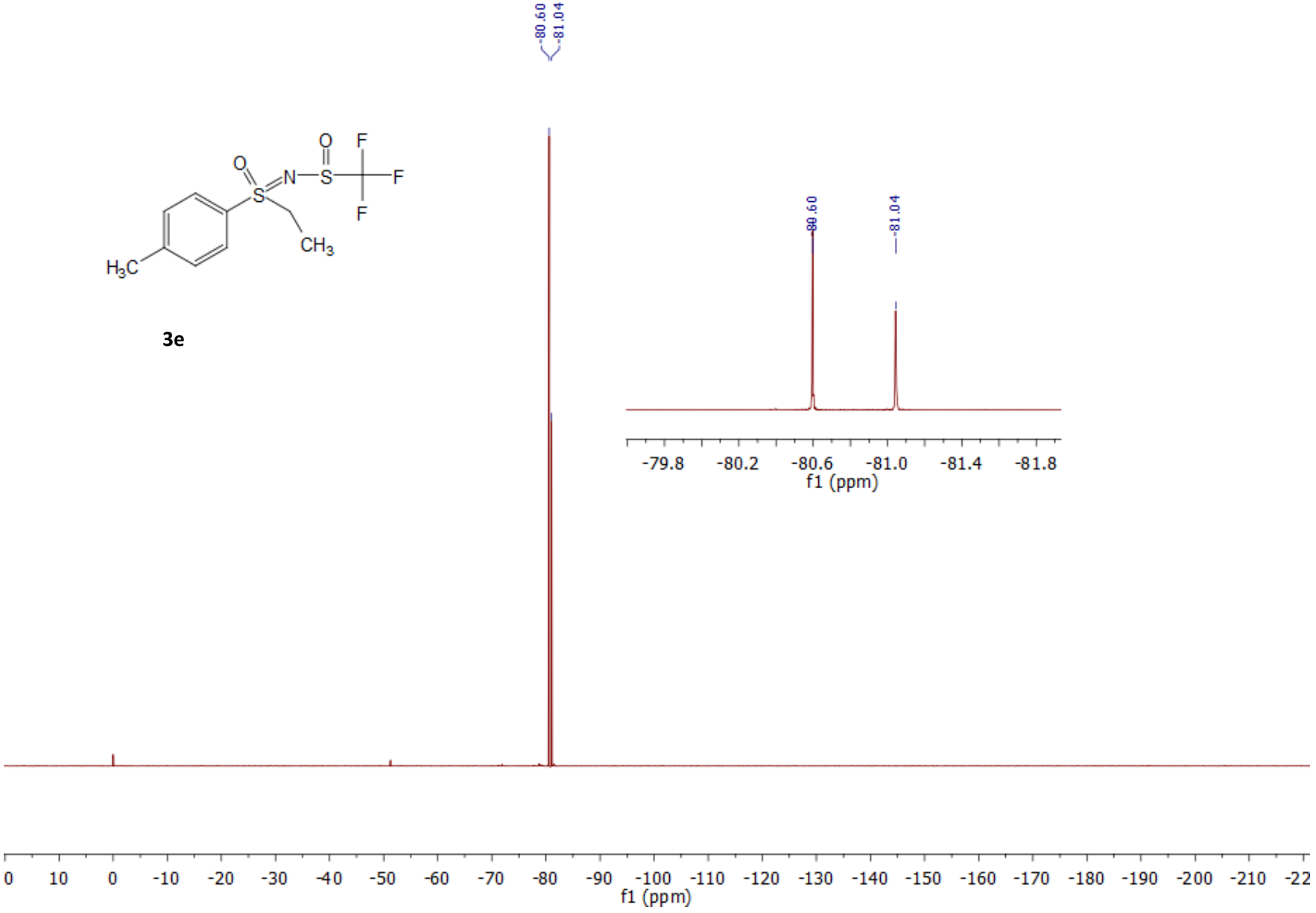
3d

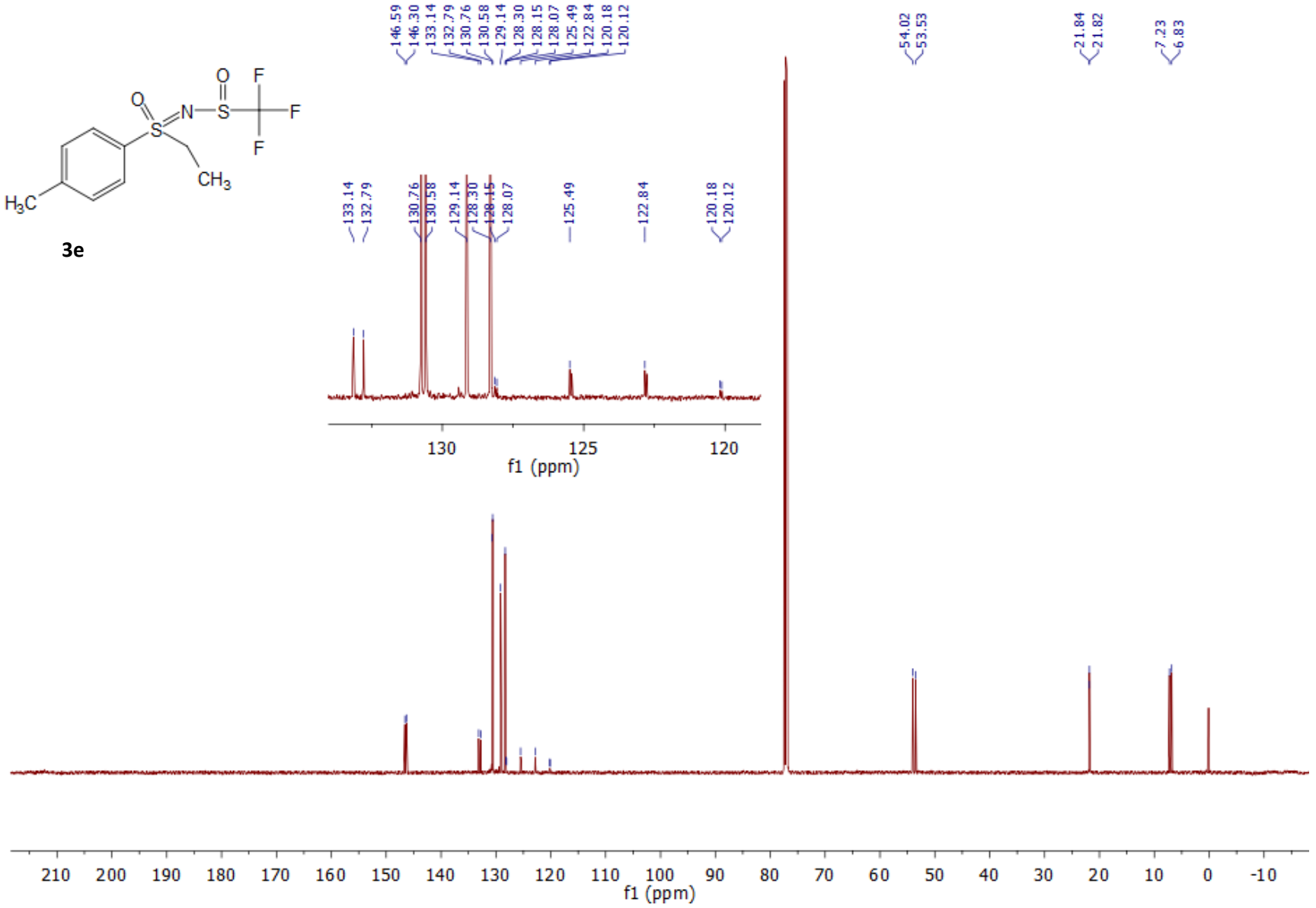

7.89
7.88
7.87
7.82
7.80
7.45
7.44
7.43
7.42
3.50
3.48
3.47
3.46
3.45
3.44
3.43
3.43
3.42
3.41
3.41
3.40
3.39
3.38
3.38
3.37
3.35
3.34
2.48
2.48
1.36
1.35
1.35
1.34
1.33
1.33
O
F
O
N
S
S
F
F
CH3
H3C
2.00
2.02
2.15
3.10
3.21
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

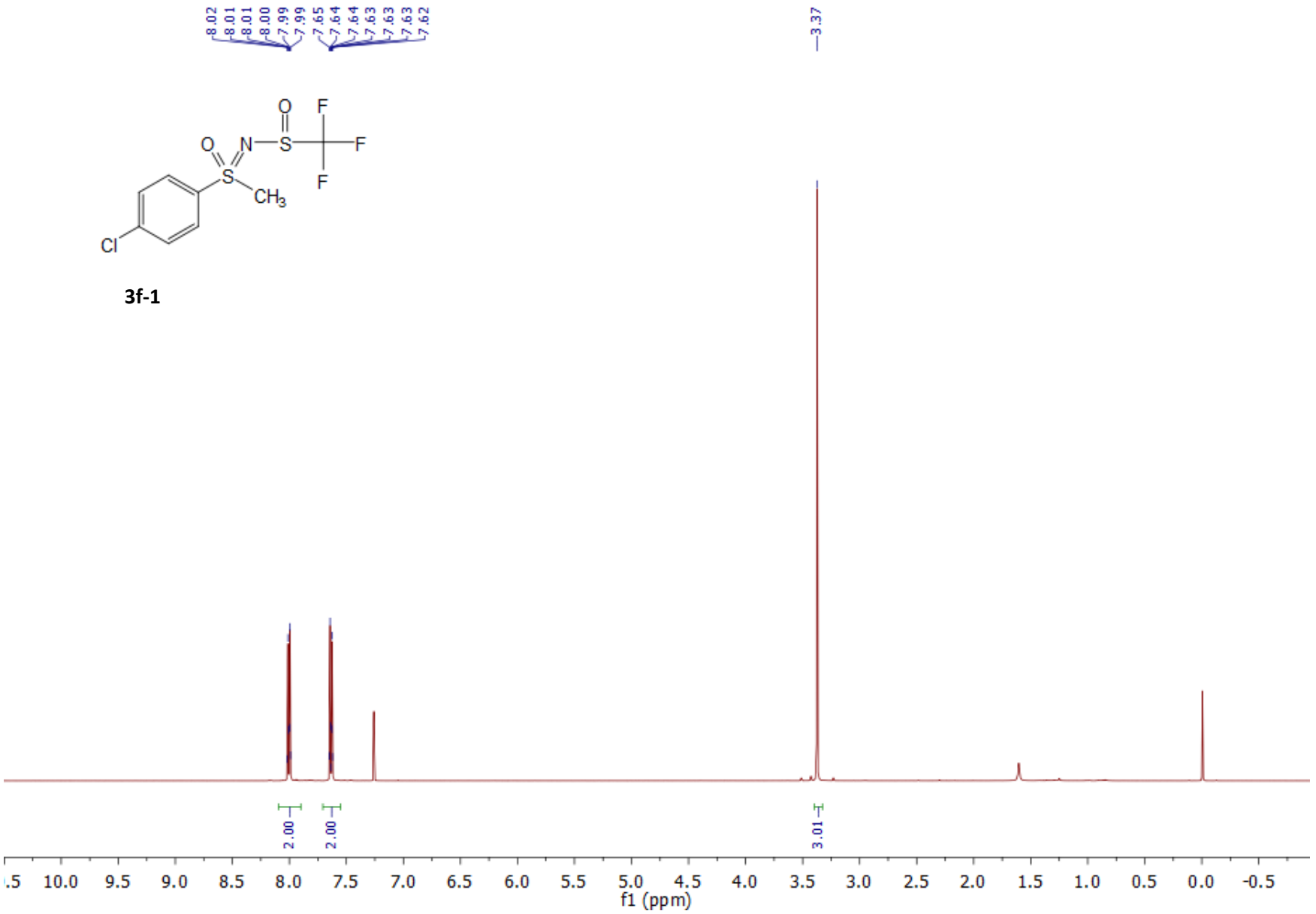
3e

O
F
O
N
S
F
S
F
CH3
H3C

3e


-80.60
-81.04
-80.60
-81.04
-79.8
-80.2
-80.6
-81.0
-81.4
-81.8
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

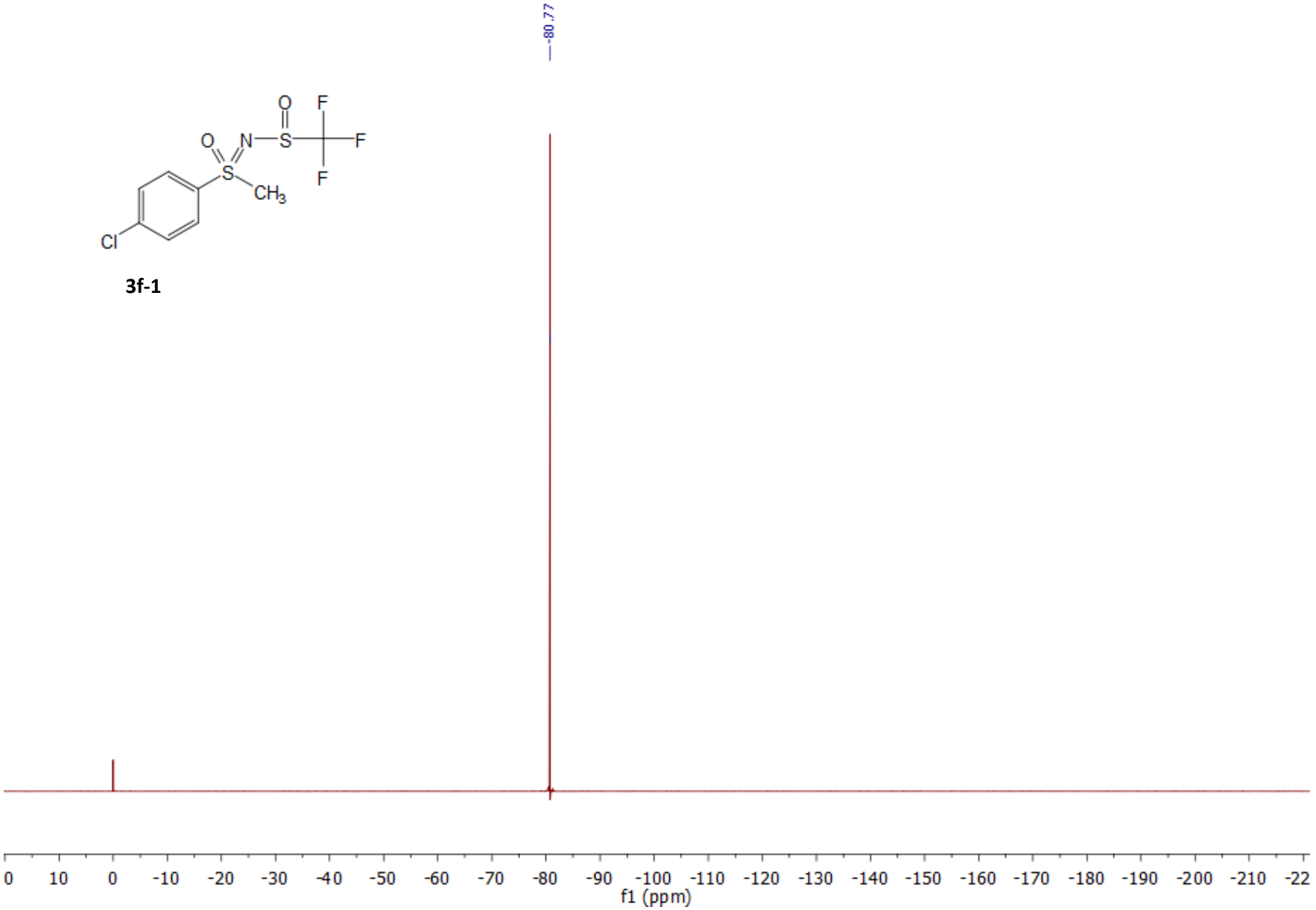

3e
146.59
146.30
133.14
132.79
130.76
130.58
129.14
128.30
128.15
128.07
125.49
122.84
120.18
120.12
54.02
53.53
21.84
21.82
7.23
6.83
f1 (ppm)
f1 (ppm)

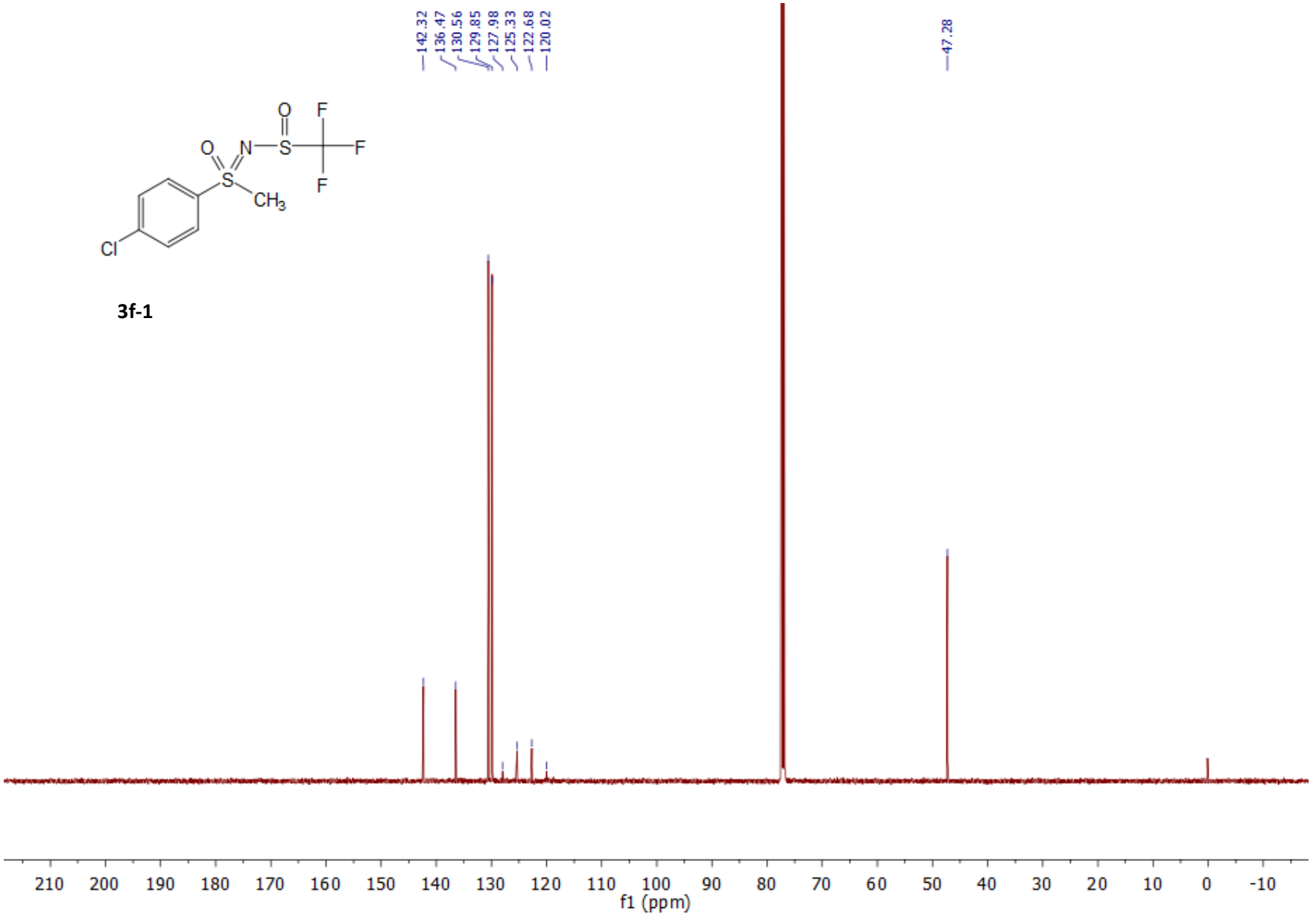

8.02
8.01
8.01
8.00
7.99
7.99
7.65
7.64
7.64
7.63
7.63
7.63
7.62
3.37
O
F
O
N
S
F
S
CH3
F
Cl
2.00
2.00
3.01
.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3f-1

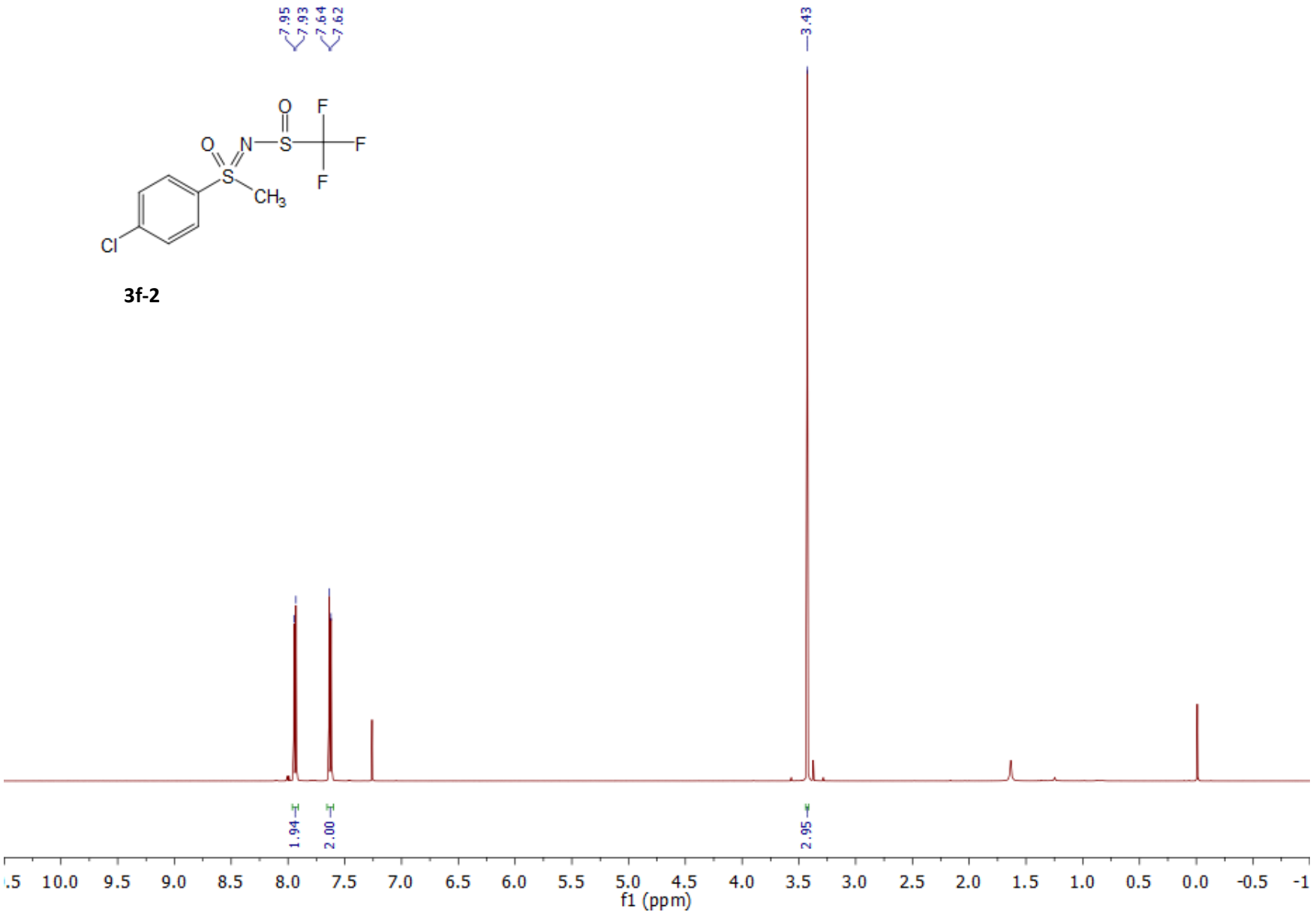
O
F
O
N
S
F
S
F
CH3
Cl

3f-1


-80.77
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


142.32
136.47
130.56
129.85
127.98
125.33
122.68
120.02
47.28
O
F
O
N
S
F
S
F
CH3
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

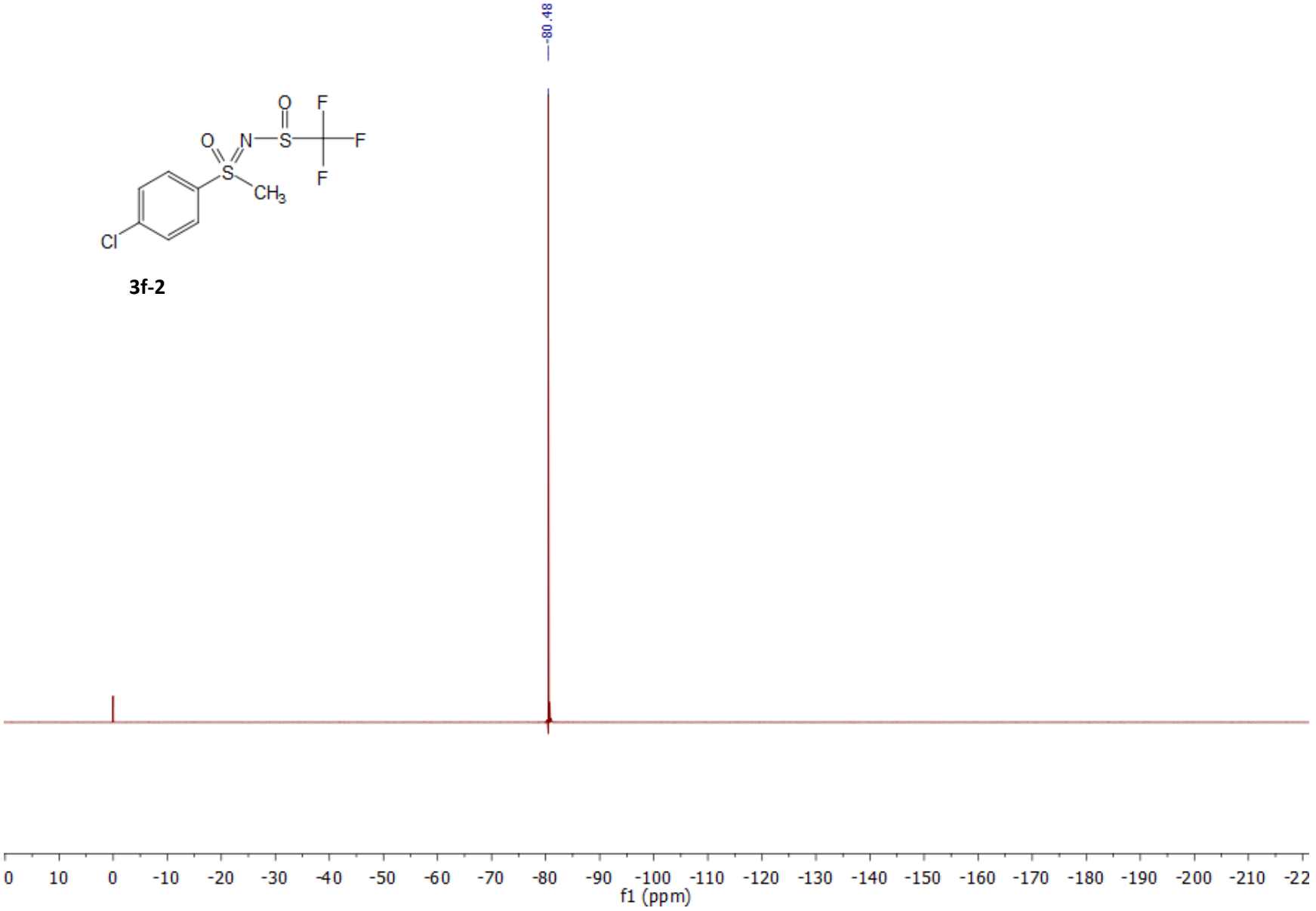
3f-1

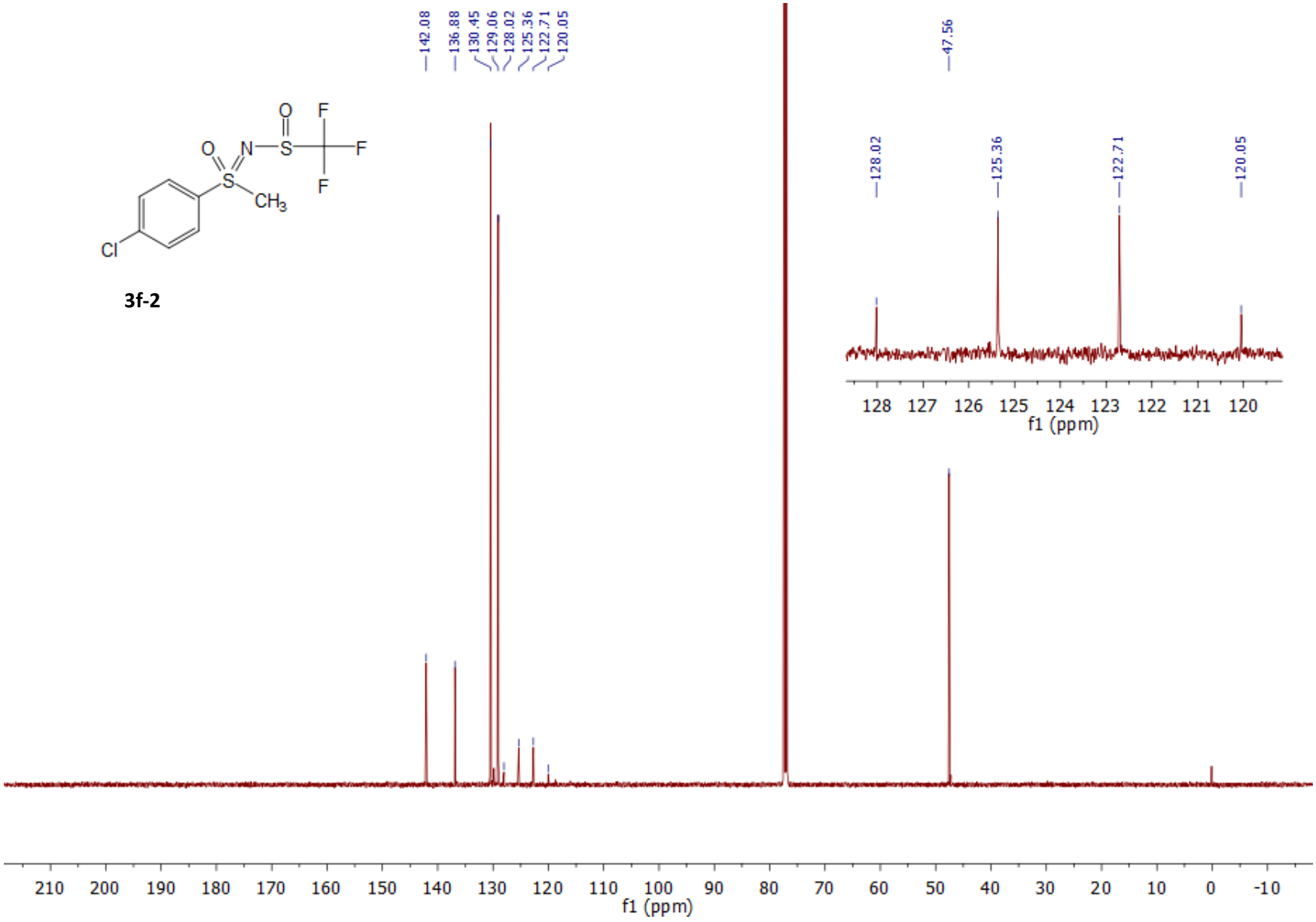

7.95
7.93
7.64
7.62
3.43
O
F
O
N
S
F
S
F
CH3
Cl
1.94
2.00
2.95
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

3f-2

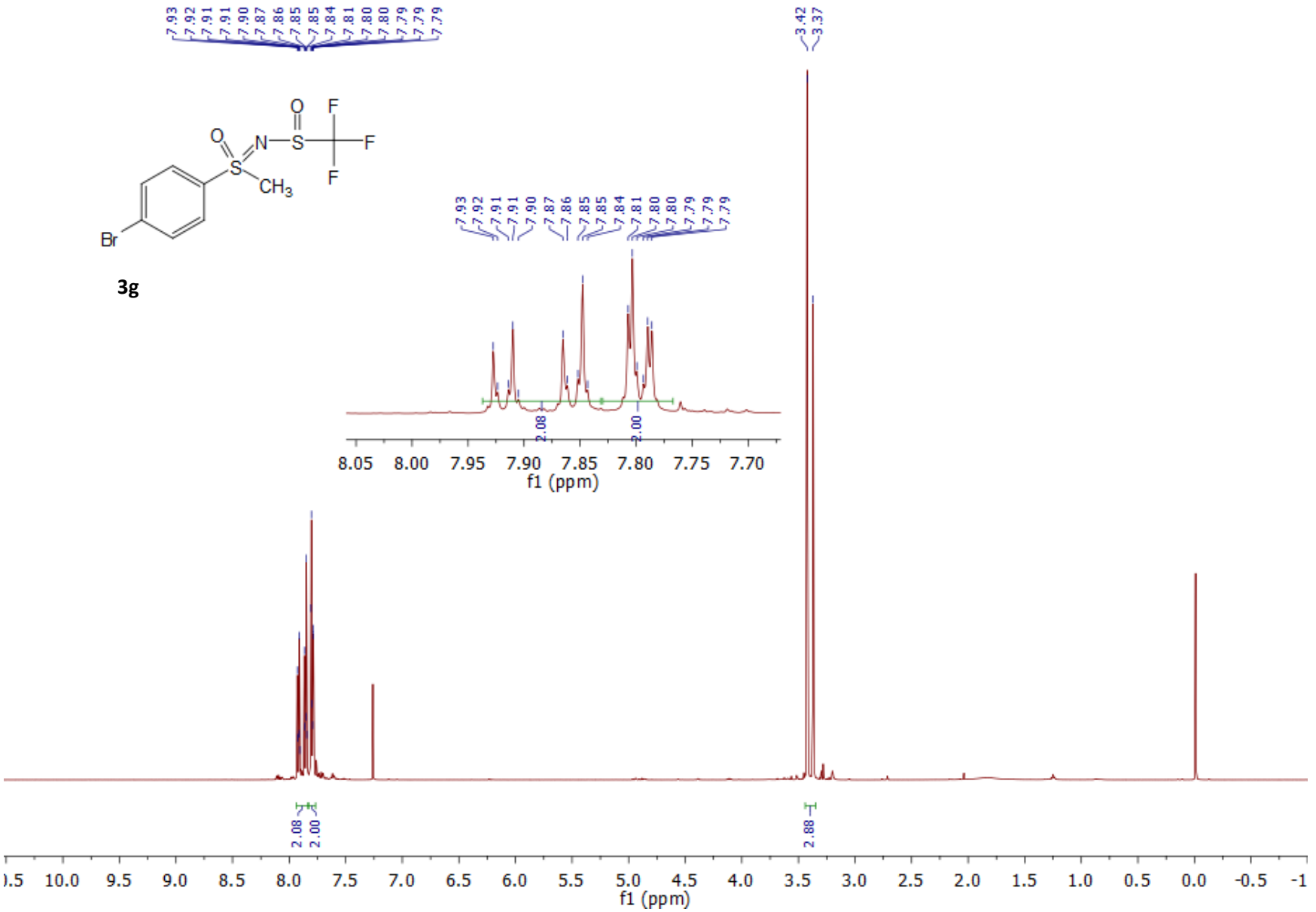
O
F
O
N
S
F
S
F
CH3
Cl

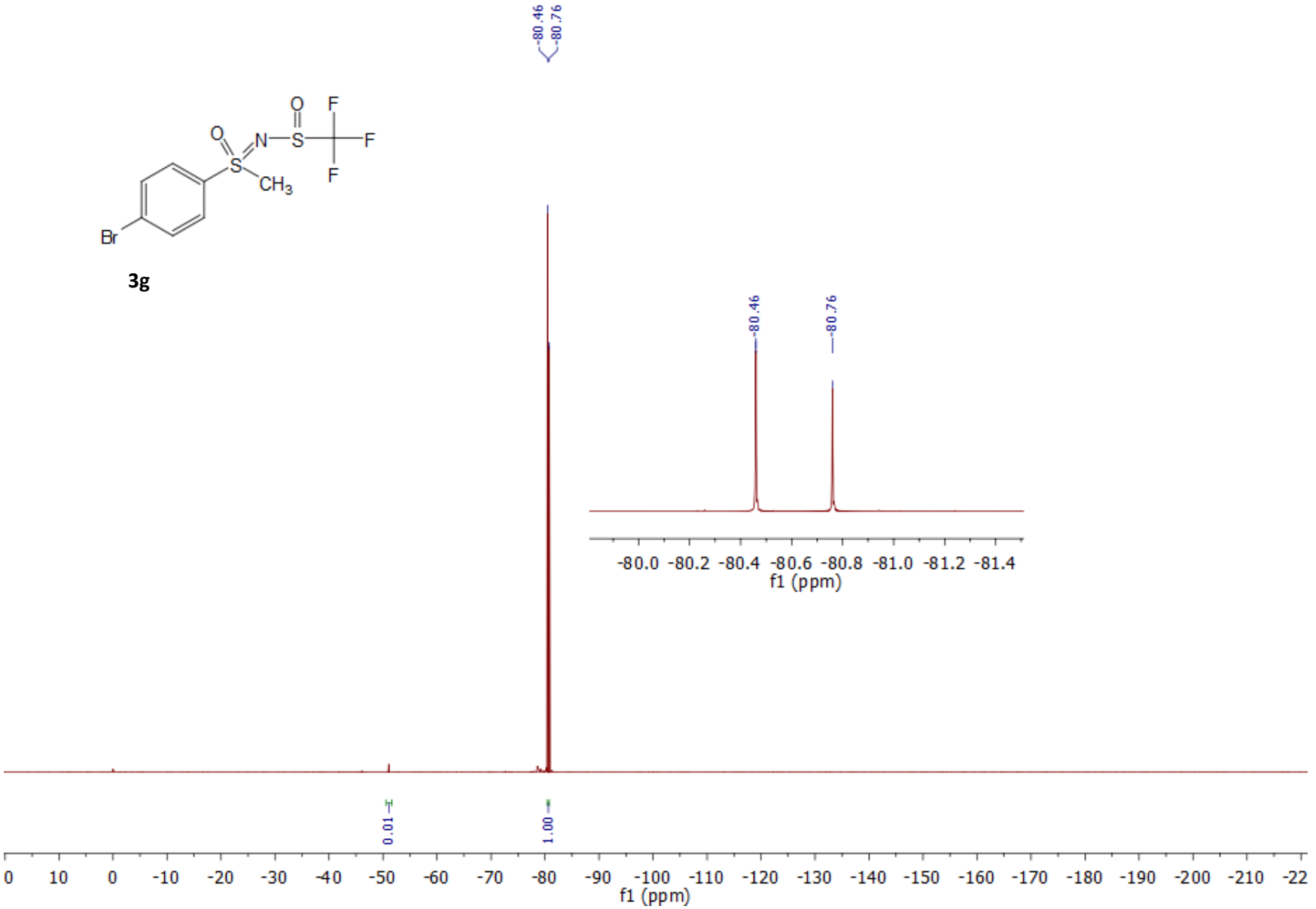
3f-2


-80.48
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

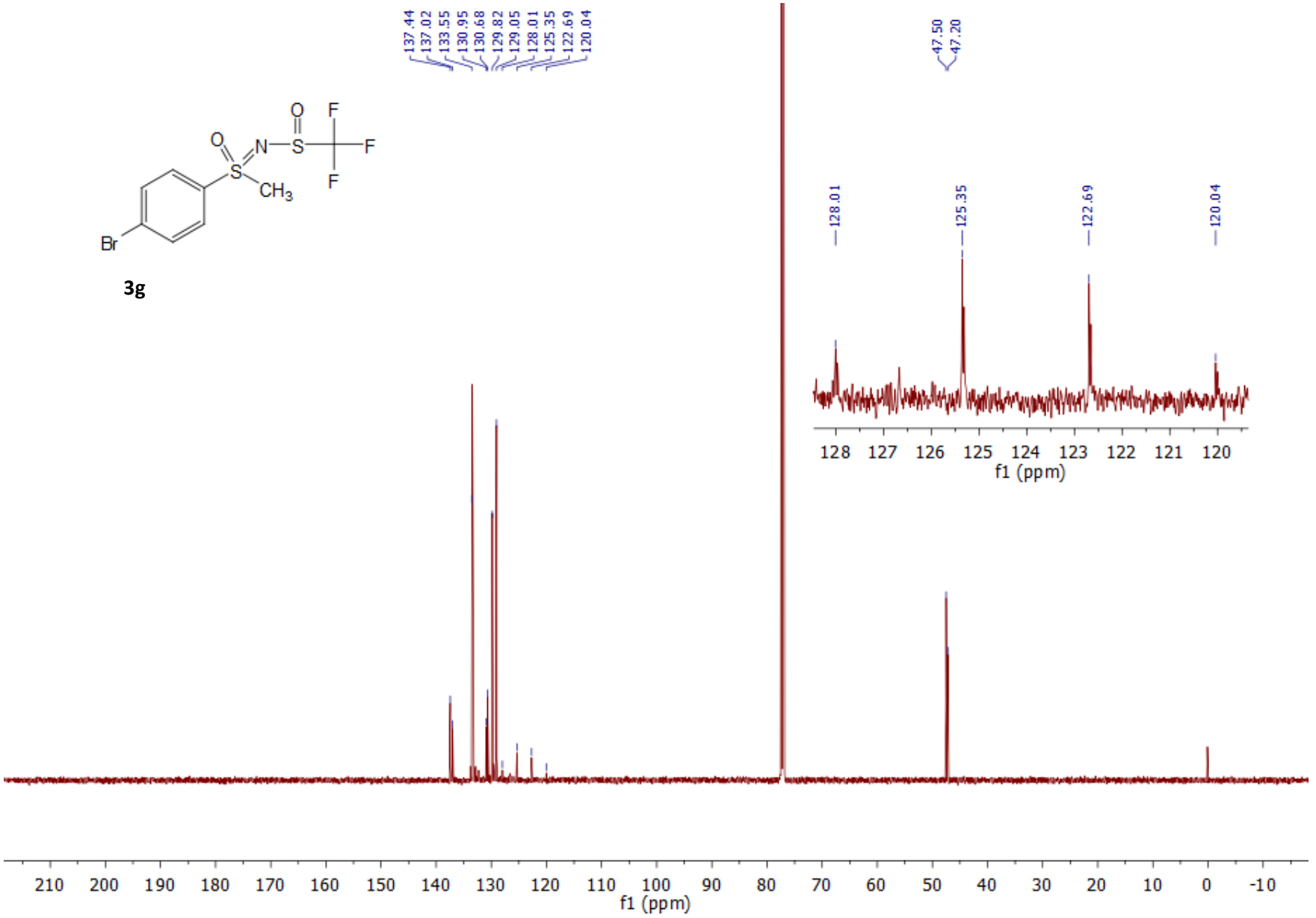

142.08
136.88
130.45
129.06
128.02
125.36
122.71
120.05
47.56
O
F
O
N
S
F
S
F
CH3
Cl
128.02
125.36
122.71
120.05
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3f-2

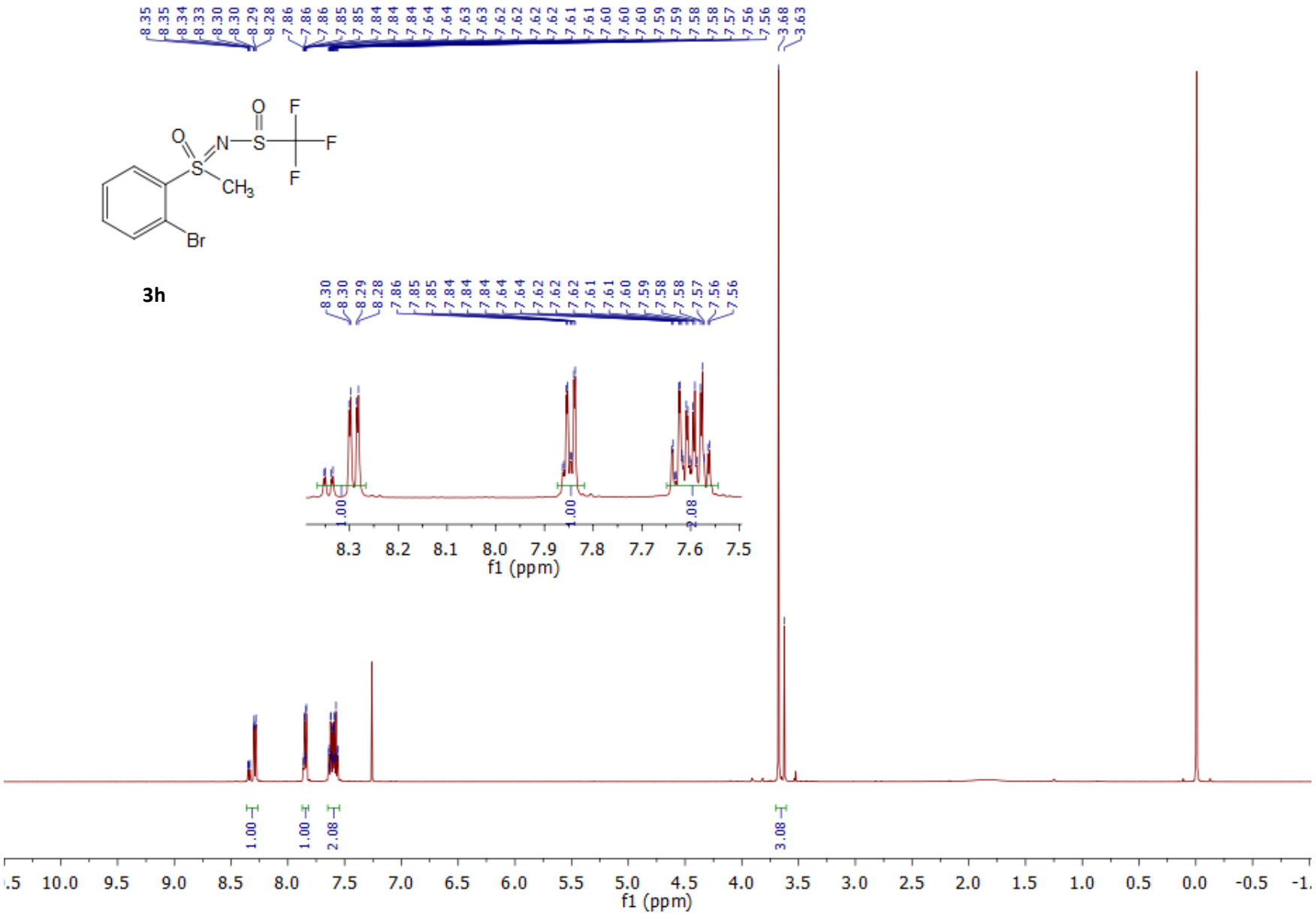

7.93
7.92
7.91
7.91
7.90
7.87
7.86
7.85
7.85
7.84
7.81
7.80
7.80
7.79
7.79
7.79
3.42
3.37
O
F
O
N
S
F
S
CH3
F
Br
3g
2.08
2.00
8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70
f1 (ppm)
2.08
2.00
2.88
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

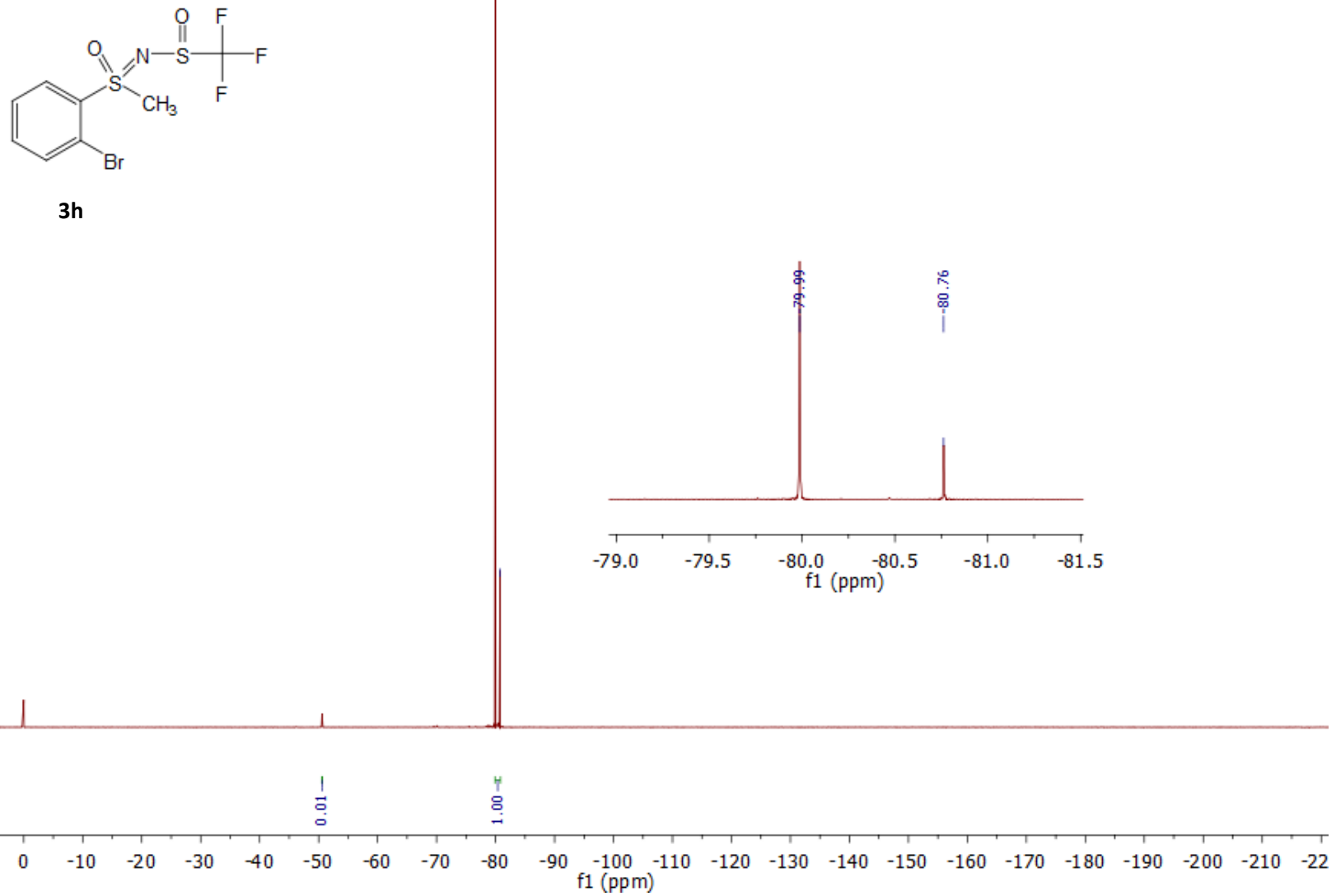

-80.46
-80.76
O
F
O
N
S
F
S
F
CH3
Br
-80.46
-80.76
-80.0 -80.2 -80.4 -80.6 -80.8 -81.0 -81.2 -81.4
f1 (ppm)
0.01
1.00
0 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)

3g

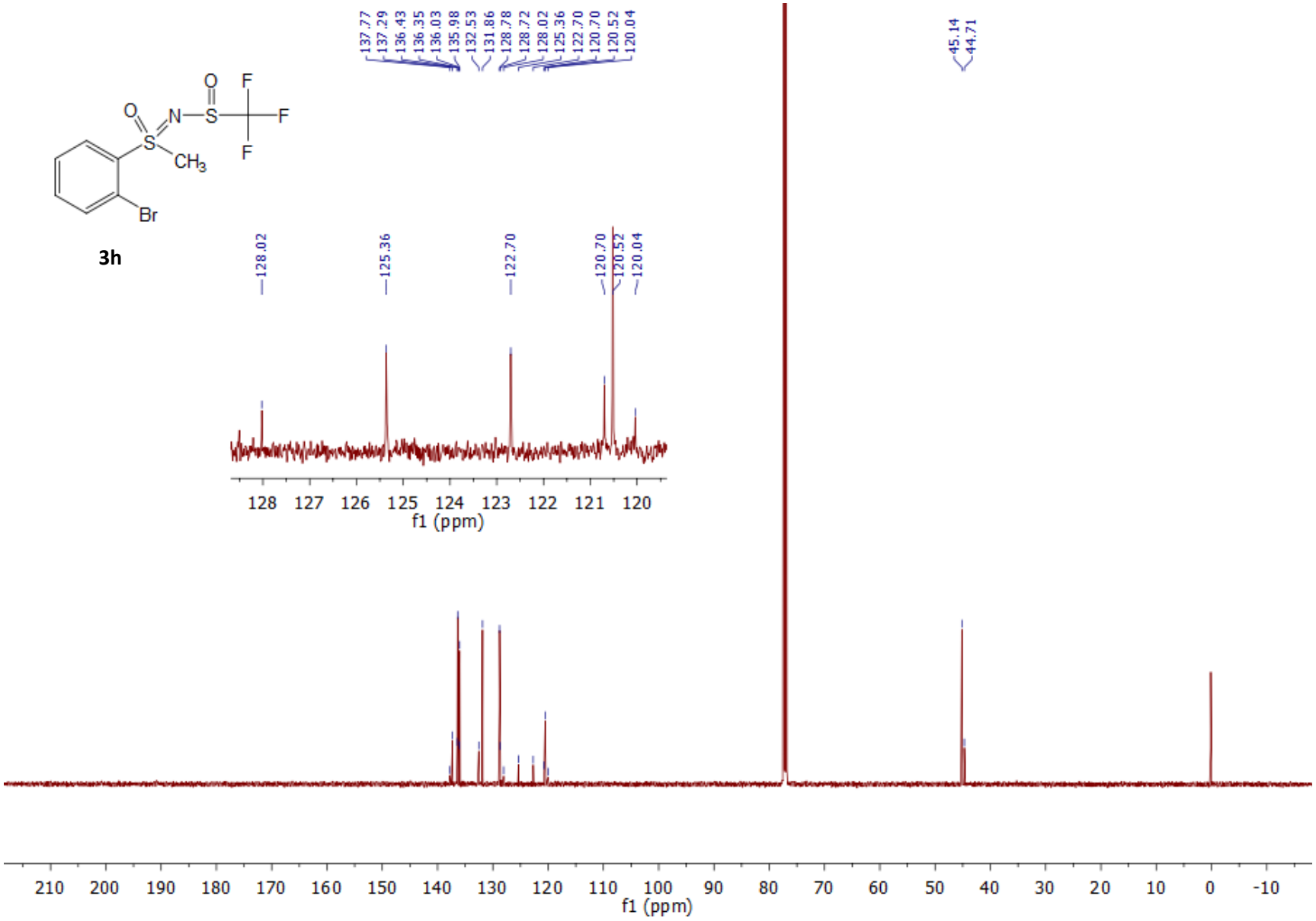

137.44
137.02
133.55
130.95
130.68
129.82
129.05
128.01
125.35
122.69
120.04
47.50
47.20
O
F
O
N
S
F
S
F
CH3
Br
128.01
125.35
122.69
120.04
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

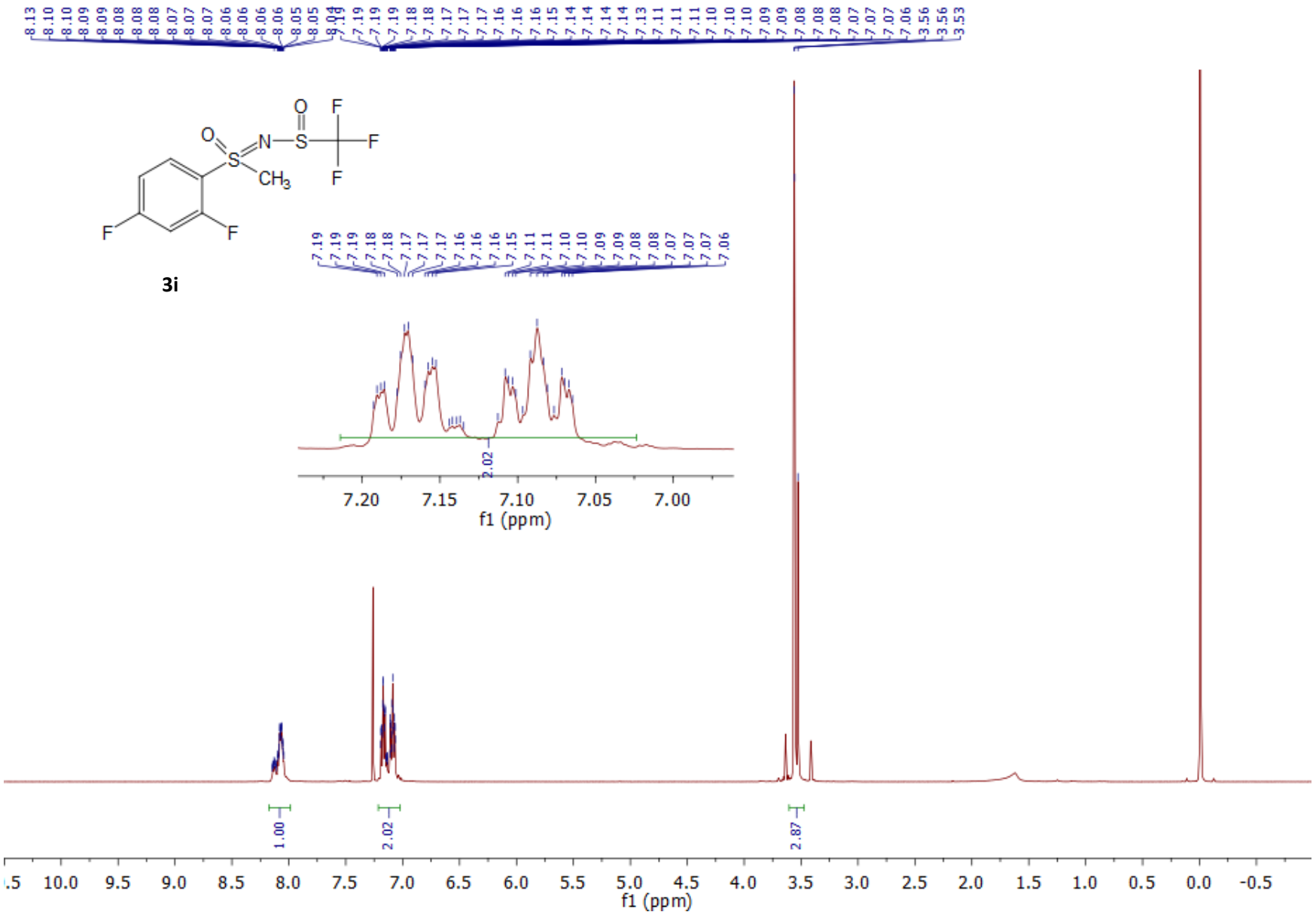
3g

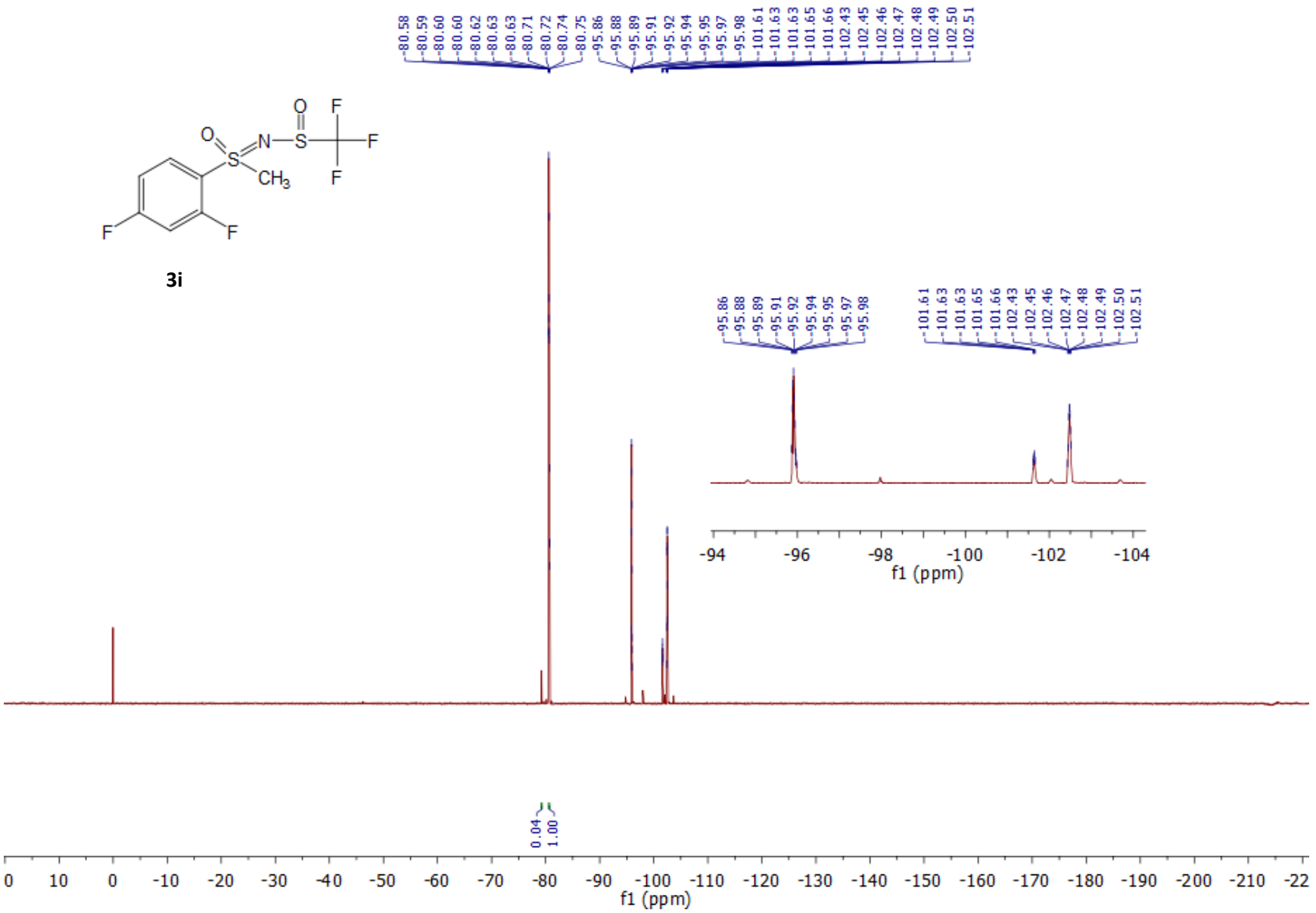

8.35 8.35 8.34 8.33 8.30 8.30 8.29 8.28 7.86 7.86 7.85 7.85 7.84 7.84 7.84 7.64 7.64 7.63 7.63 7.62 7.62 7.62 7.62 7.61 7.61 7.60 7.60 7.60 7.59 7.59 7.58 7.58 7.57 7.56 7.56 3.68 3.63
O F
O N S F
S F
CH3
Br
3h
8.30 8.30 8.29 8.28 7.86 7.85 7.84 7.84 7.84 7.64 7.64 7.62 7.62 7.62 7.61 7.61 7.60 7.59 7.58 7.58 7.57 7.56 7.56
1.00 1.00 2.08
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
f1 (ppm)
1.00 1.00 2.08 3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

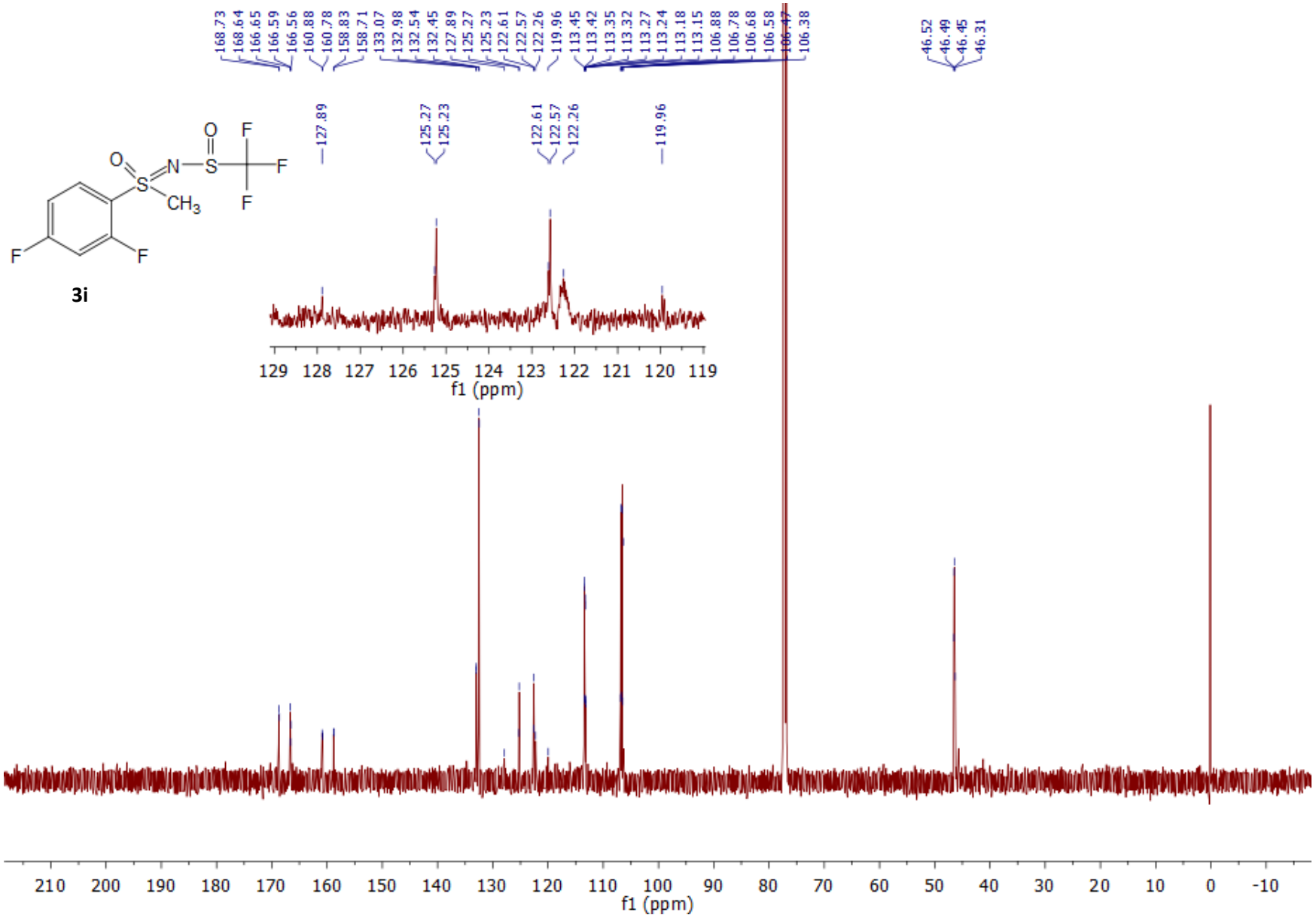

-79.99
-80.76
O
F
O
N
S
F
S
F
CH3
Br
-79.99
-80.76
-79.0
-79.5
-80.0
-80.5
-81.0
-81.5
f1 (ppm)
0.01
1.00
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

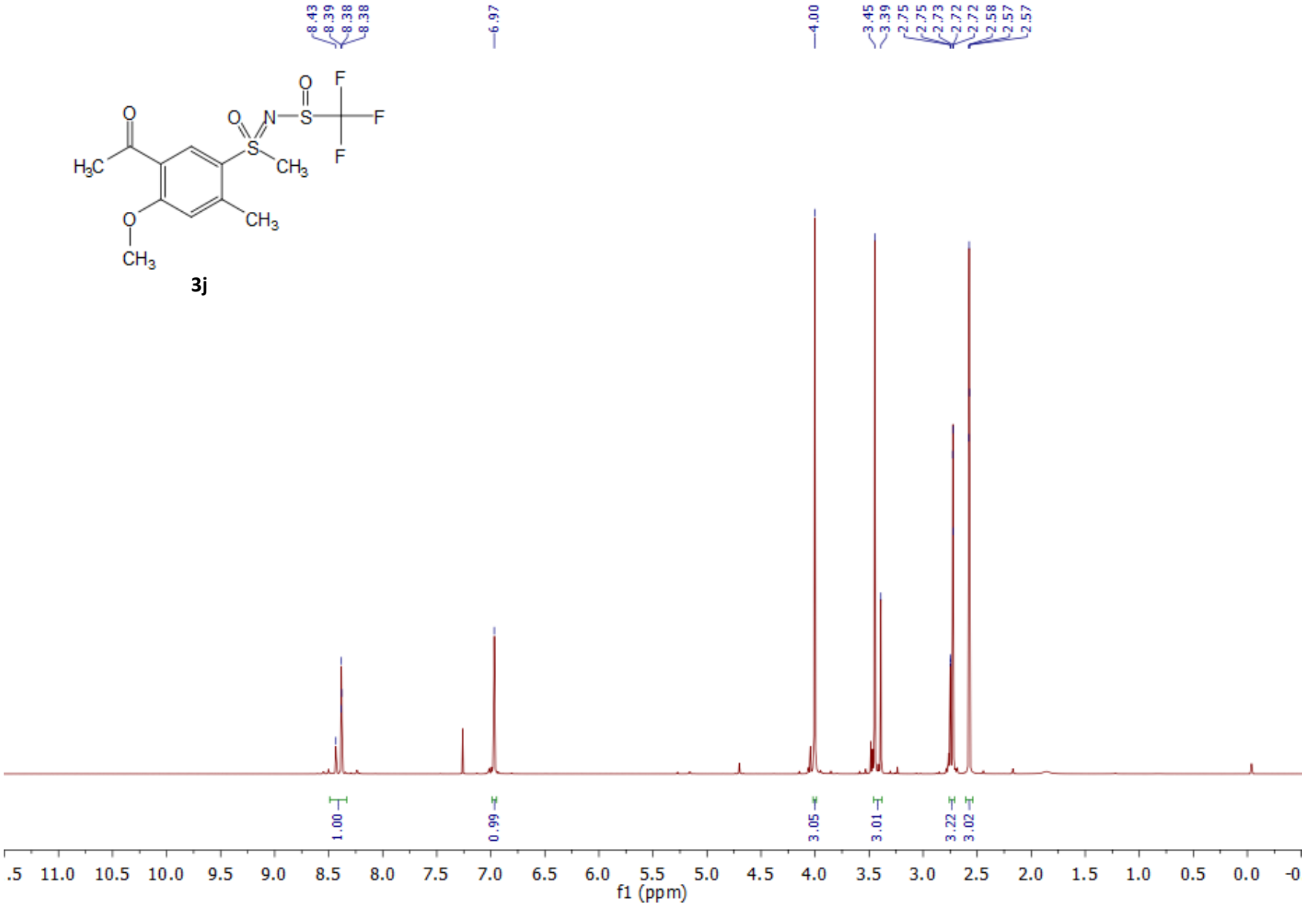
3h


137.77
137.29
136.43
136.35
136.03
135.98
132.53
131.86
128.78
128.72
128.02
125.36
122.70
120.70
120.52
120.04
45.14
44.71
O
F
O
N
S
F
S
CH3
F
Br
3h
128.02
125.36
122.70
120.70
120.52
120.04
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

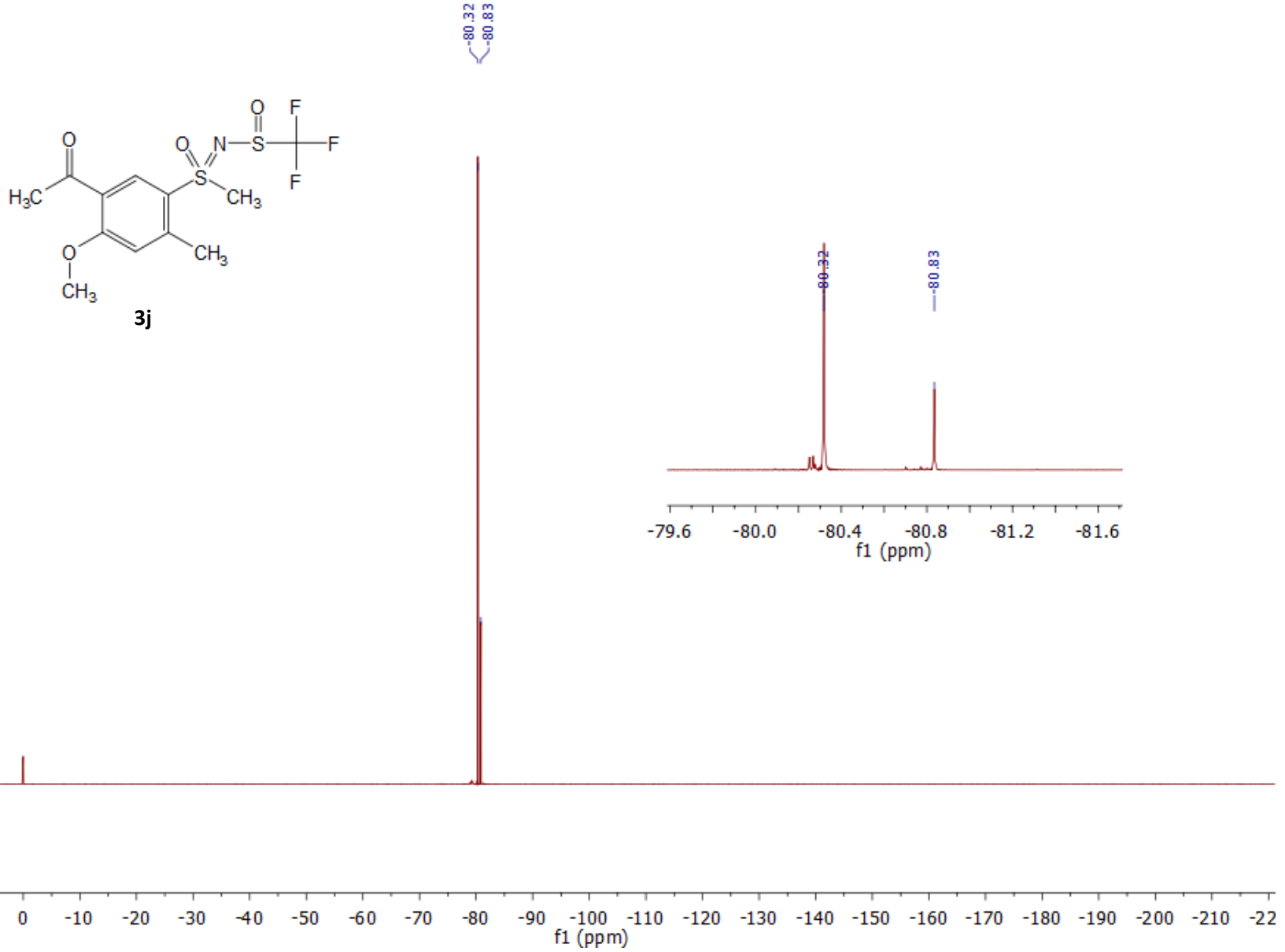

3i
7.20
7.15
7.10
7.05
7.00
f1 (ppm)
2.02
1.00
2.02
2.87
f1 (ppm)


-80.58
-80.59
-80.60
-80.60
-80.62
-80.63
-80.63
-80.71
-80.72
-80.74
-80.75
-95.86
-95.88
-95.89
-95.91
-95.92
-95.94
-95.95
-95.97
-95.98
-101.61
-101.63
-101.63
-101.65
-101.66
-102.43
-102.45
-102.46
-102.47
-102.48
-102.49
-102.50
-102.51
O
F
O
N
S
F
S
CH3
F
F
3i
-95.86
-95.88
-95.89
-95.91
-95.92
-95.94
-95.95
-95.97
-95.98
-101.61
-101.63
-101.63
-101.65
-101.66
-102.43
-102.45
-102.46
-102.47
-102.48
-102.49
-102.50
-102.51
-94
-96
-98
-100
-102
-104
f1 (ppm)
0.04
1.00
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

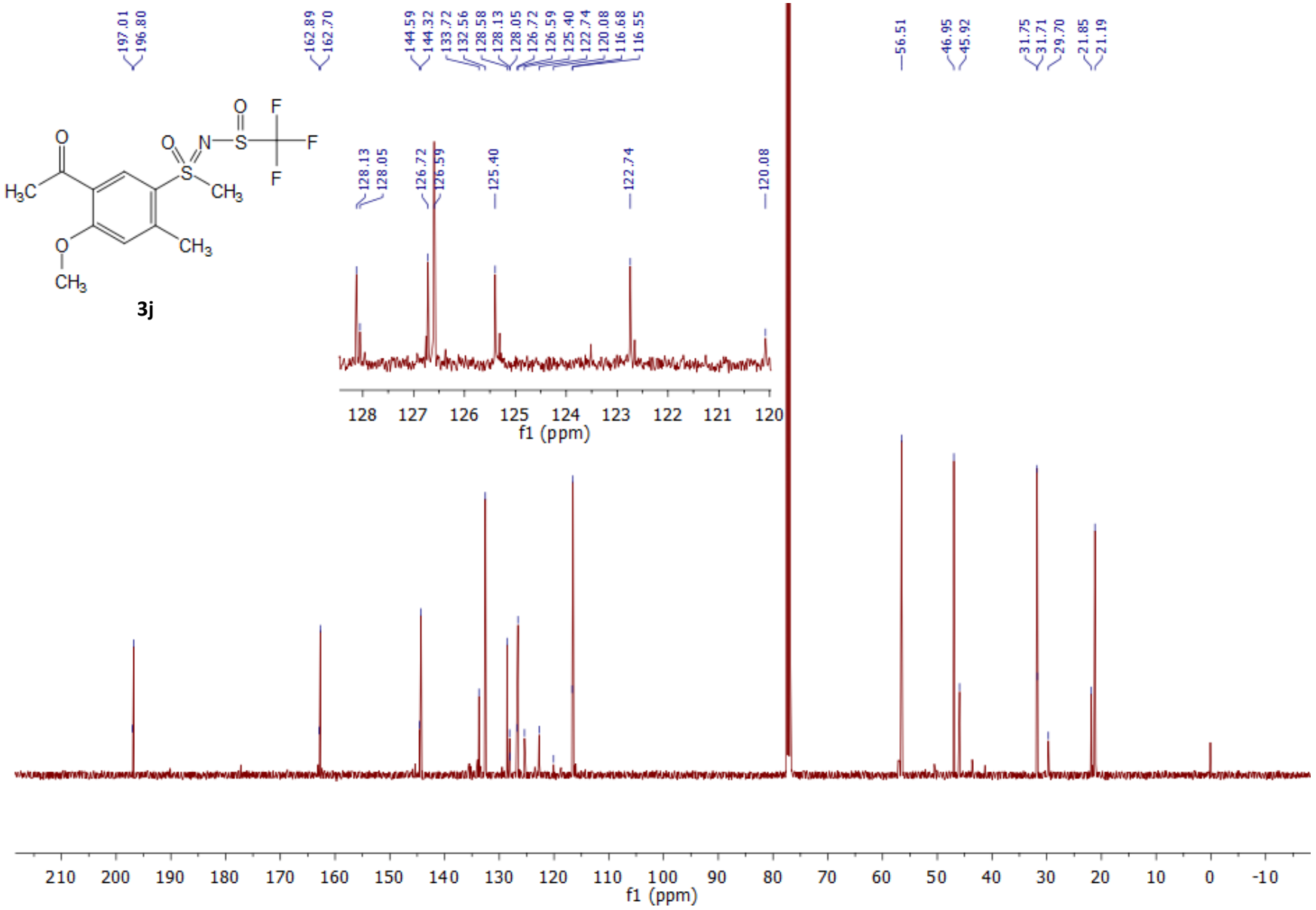

168.73
168.64
166.65
166.59
166.56
160.88
160.78
158.83
158.71
133.07
132.98
132.54
132.45
127.89
125.27
125.23
122.61
122.57
122.26
119.96
113.45
113.42
113.35
113.32
113.27
113.24
113.18
113.15
106.88
106.78
106.68
106.58
106.47
106.38
46.52
46.49
46.45
46.31
O
F
N
S
F
O
S
CH3
F
F
3i
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

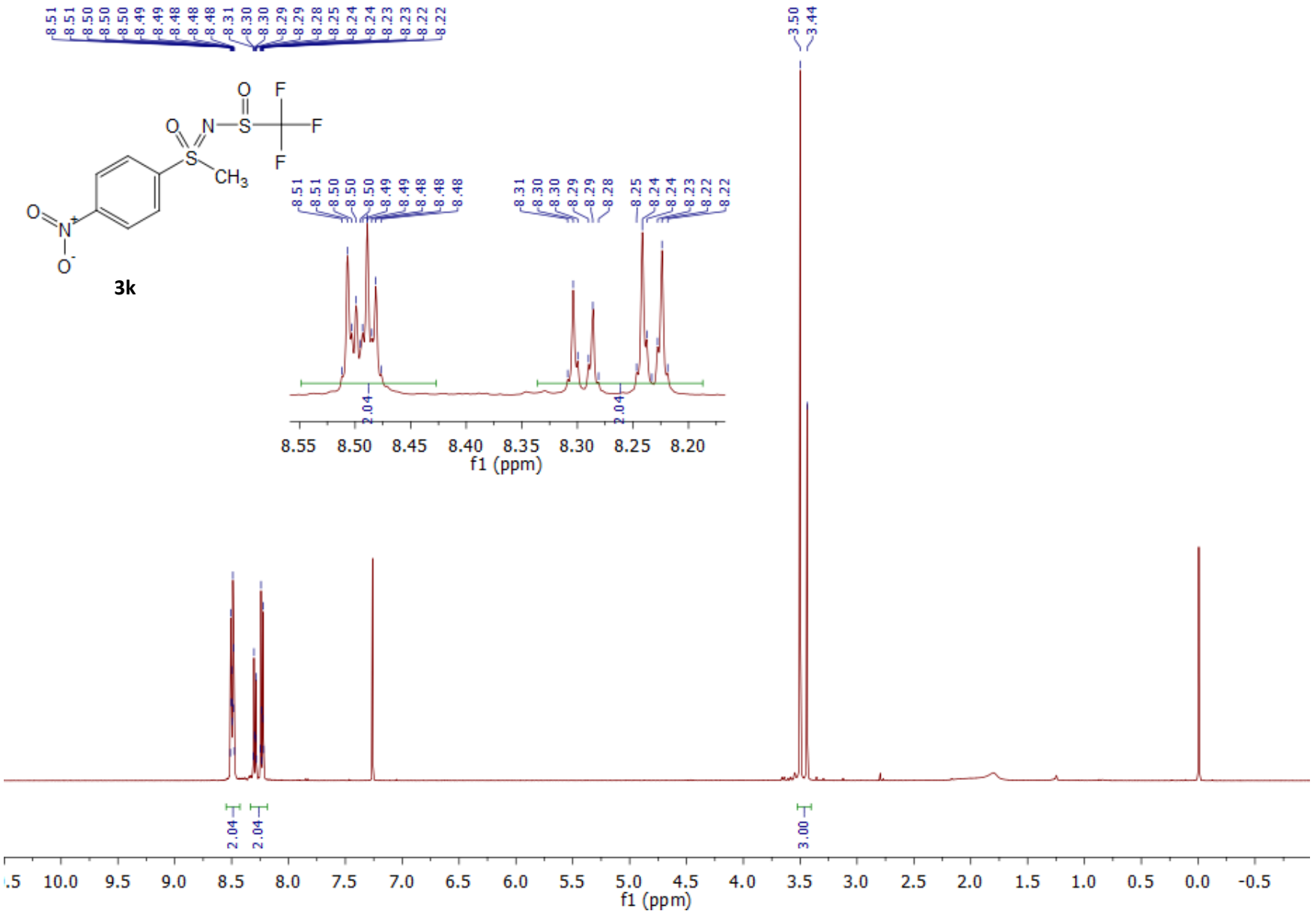

8.43
8.39
8.38
8.38
6.97
4.00
3.45
3.39
2.75
2.75
2.73
2.72
2.72
2.58
2.57
2.57
O
H3C
O
N
S
O
F
F
F
S
CH3
O
CH3
CH3
1.00
0.99
3.05
3.01
3.22
3.02
.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

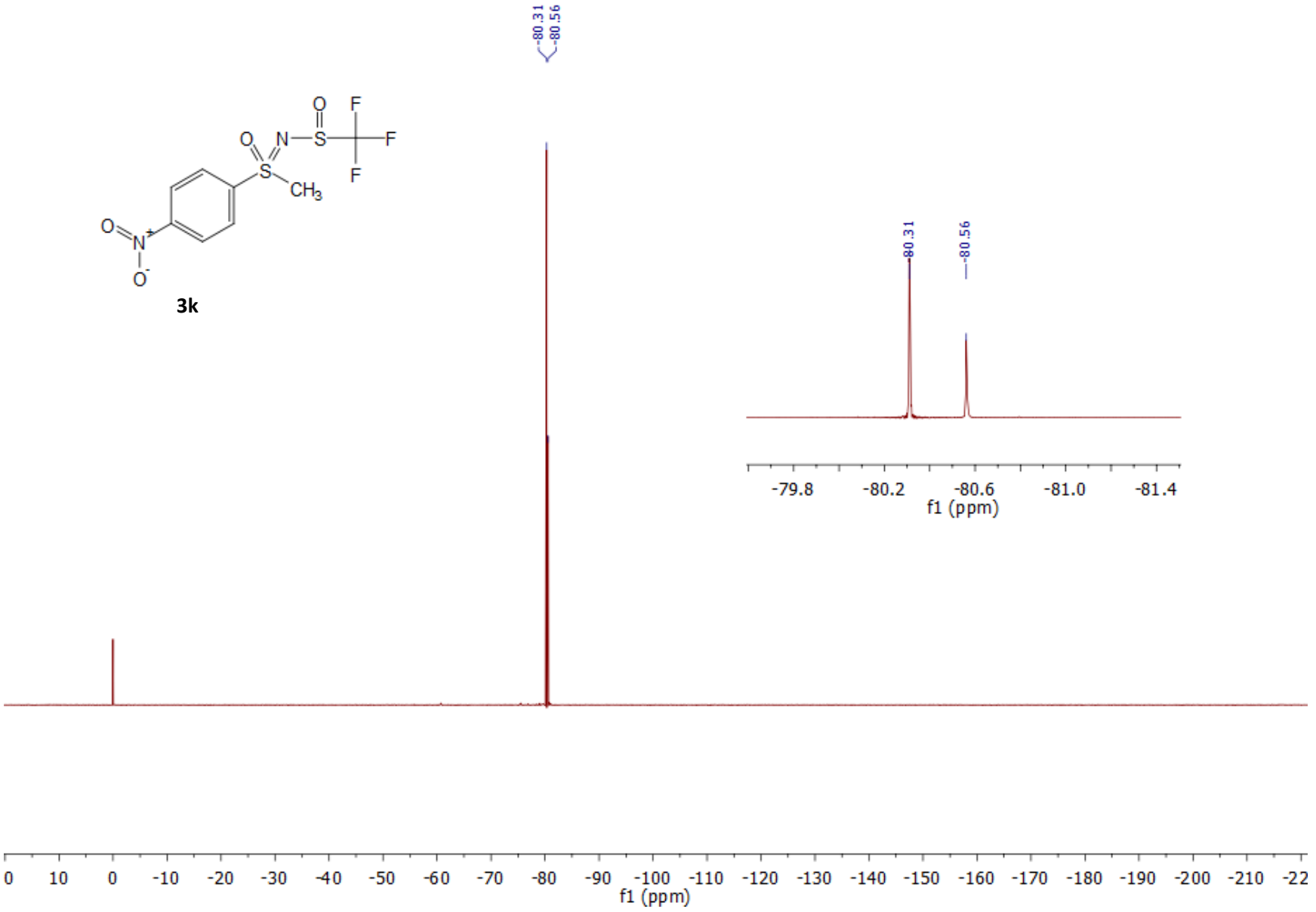
3j

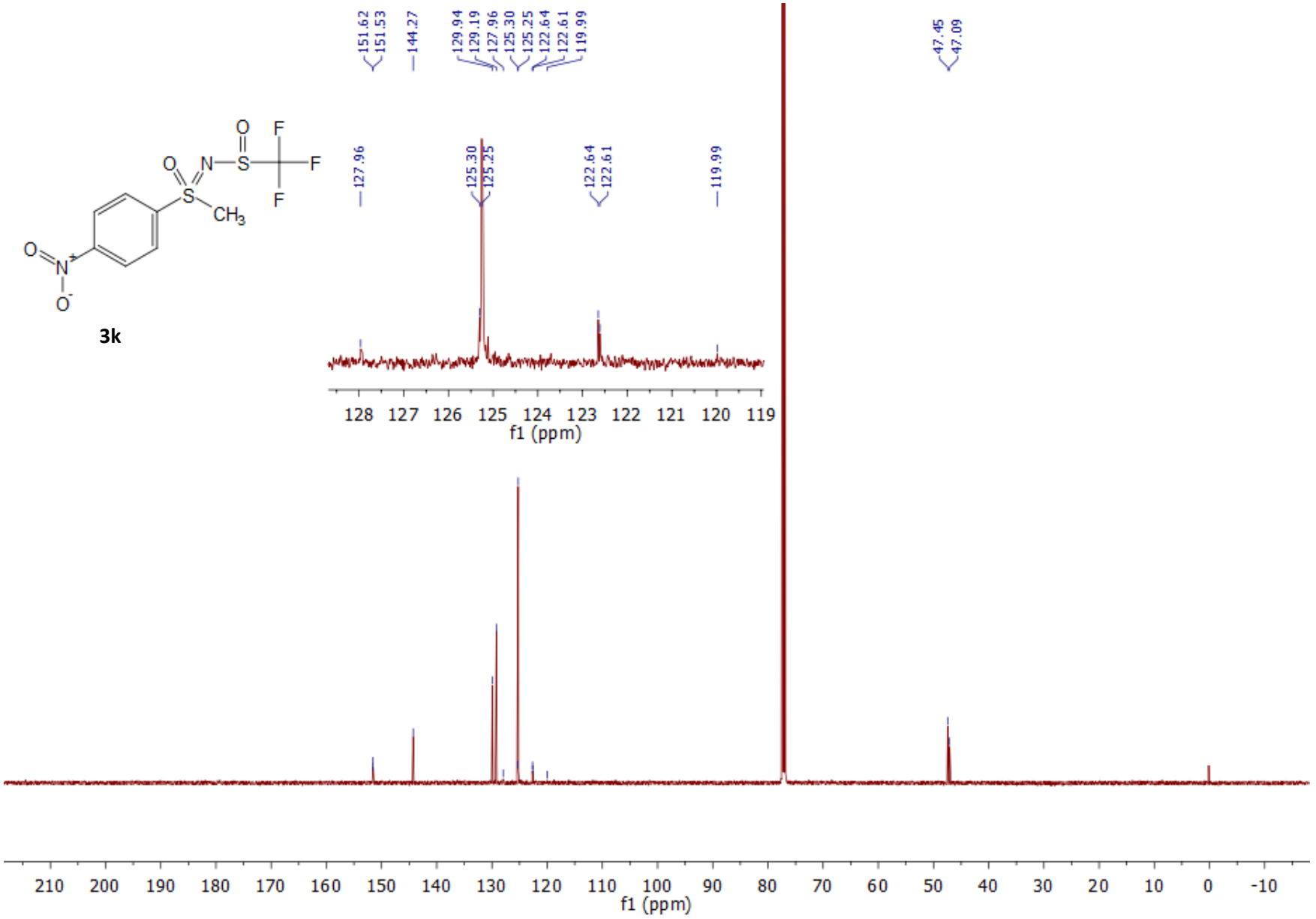

-80.32
-80.83
O
F
O
N
S
F
F
H3C
S
CH3
O
CH3
CH3
-80.32
-80.83
-79.6
-80.0
-80.4
-80.8
-81.2
-81.6
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

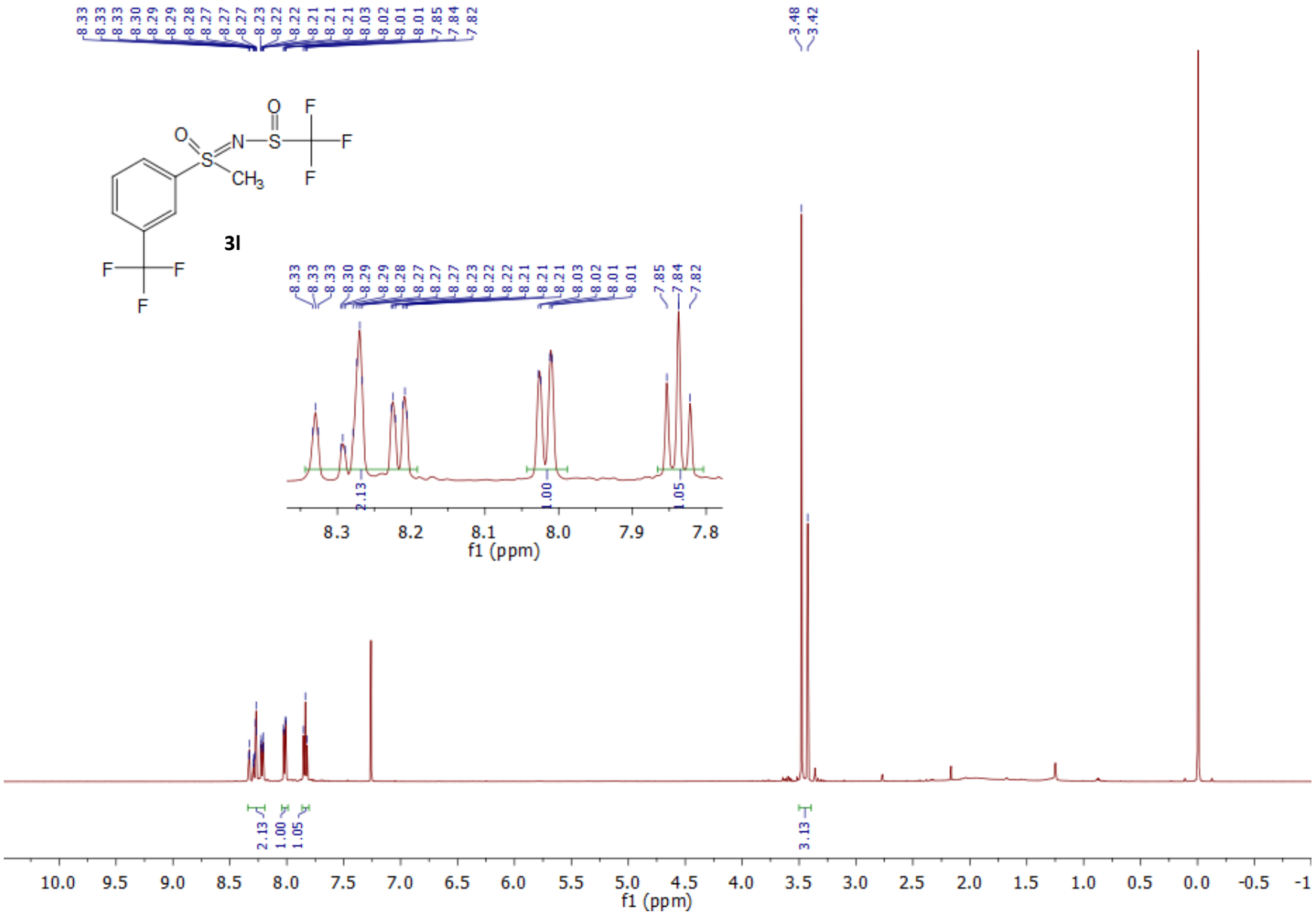
3j

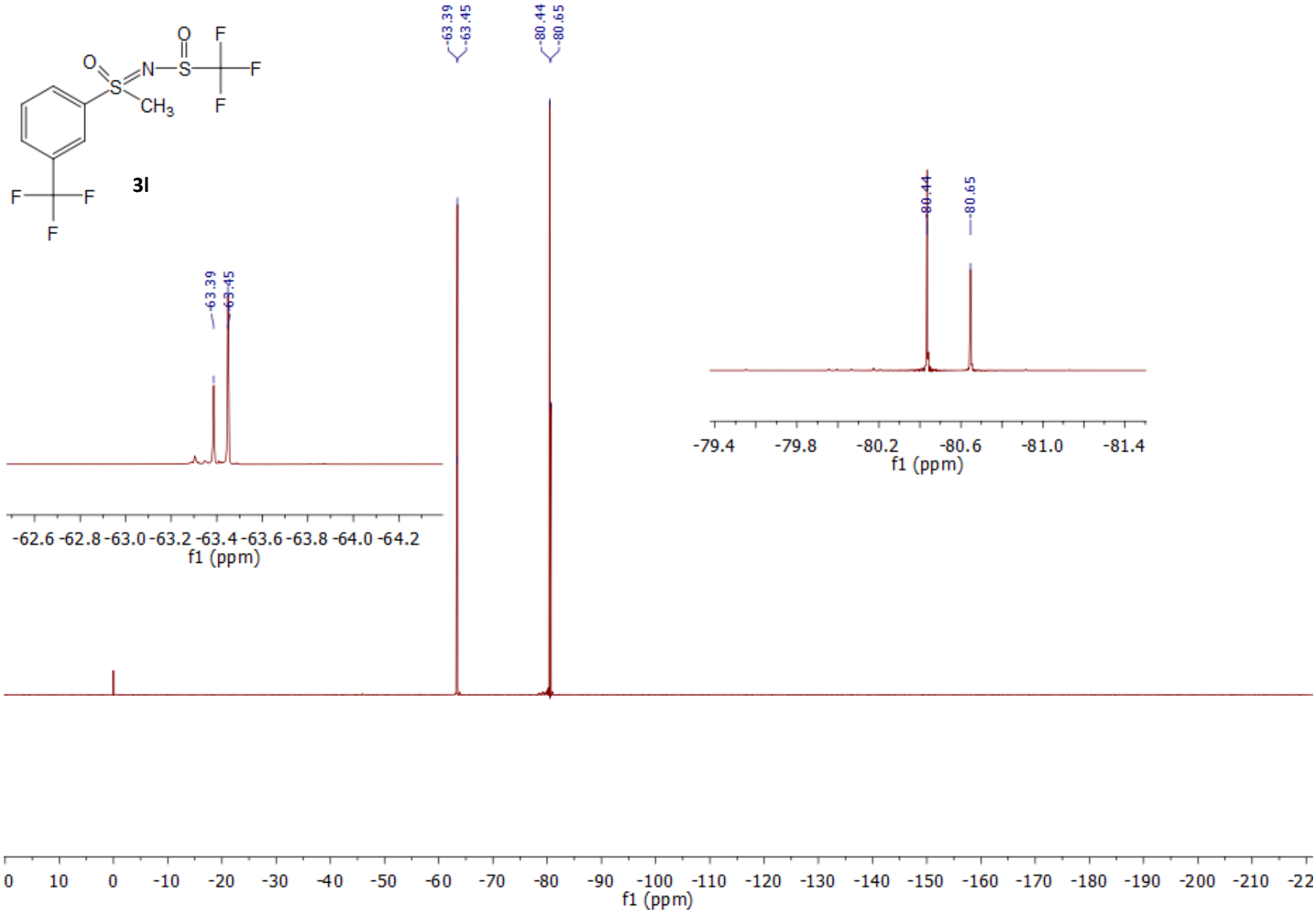

197.01
196.80
162.89
162.70
144.59
144.32
133.72
132.56
128.58
128.13
128.05
126.72
126.59
125.40
122.74
120.08
116.68
116.55
56.51
46.95
45.92
31.75
31.71
29.70
21.85
21.19
O
F
O
N
S
F
O
S
F
H3C
CH3
O
CH3
CH3
3j
f1 (ppm)
f1 (ppm)

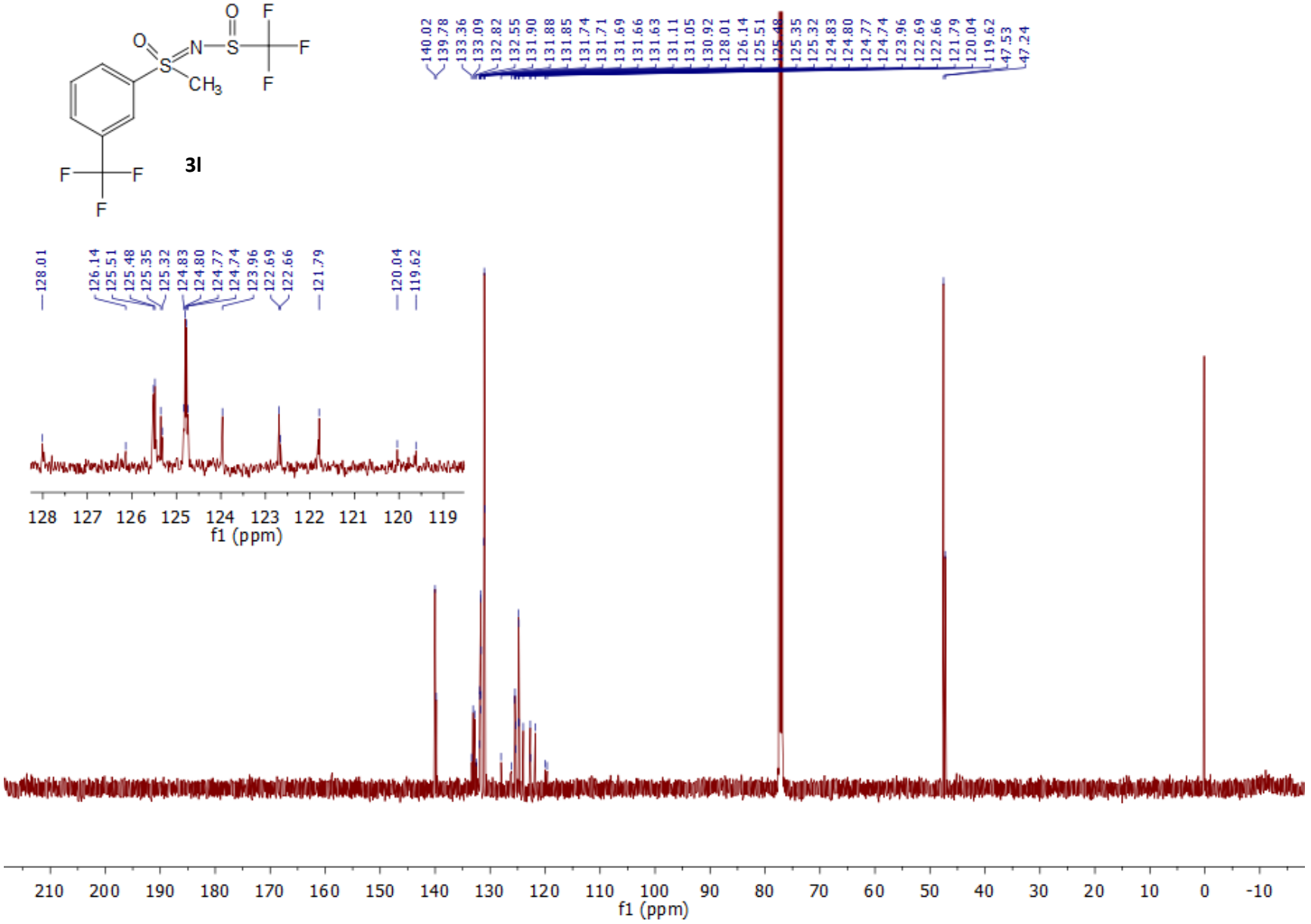

8.51 8.51 8.50 8.50 8.50 8.49 8.48 8.48 8.48 8.31 8.30 8.30 8.29 8.29 8.28 8.25 8.24 8.24 8.23 8.23 8.22 8.22
3.50 3.44
O F
O N S F
S F
CH3
O
N+
O-
3k
8.51 8.51 8.50 8.50 8.50 8.49 8.49 8.48 8.48 8.48
8.31 8.30 8.30 8.29 8.29 8.28 8.25 8.24 8.24 8.23 8.22 8.22
2.04
2.04
8.55 8.50 8.45 8.40 8.35 8.30 8.25 8.20
f1 (ppm)
2.04
2.04
3.00
.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

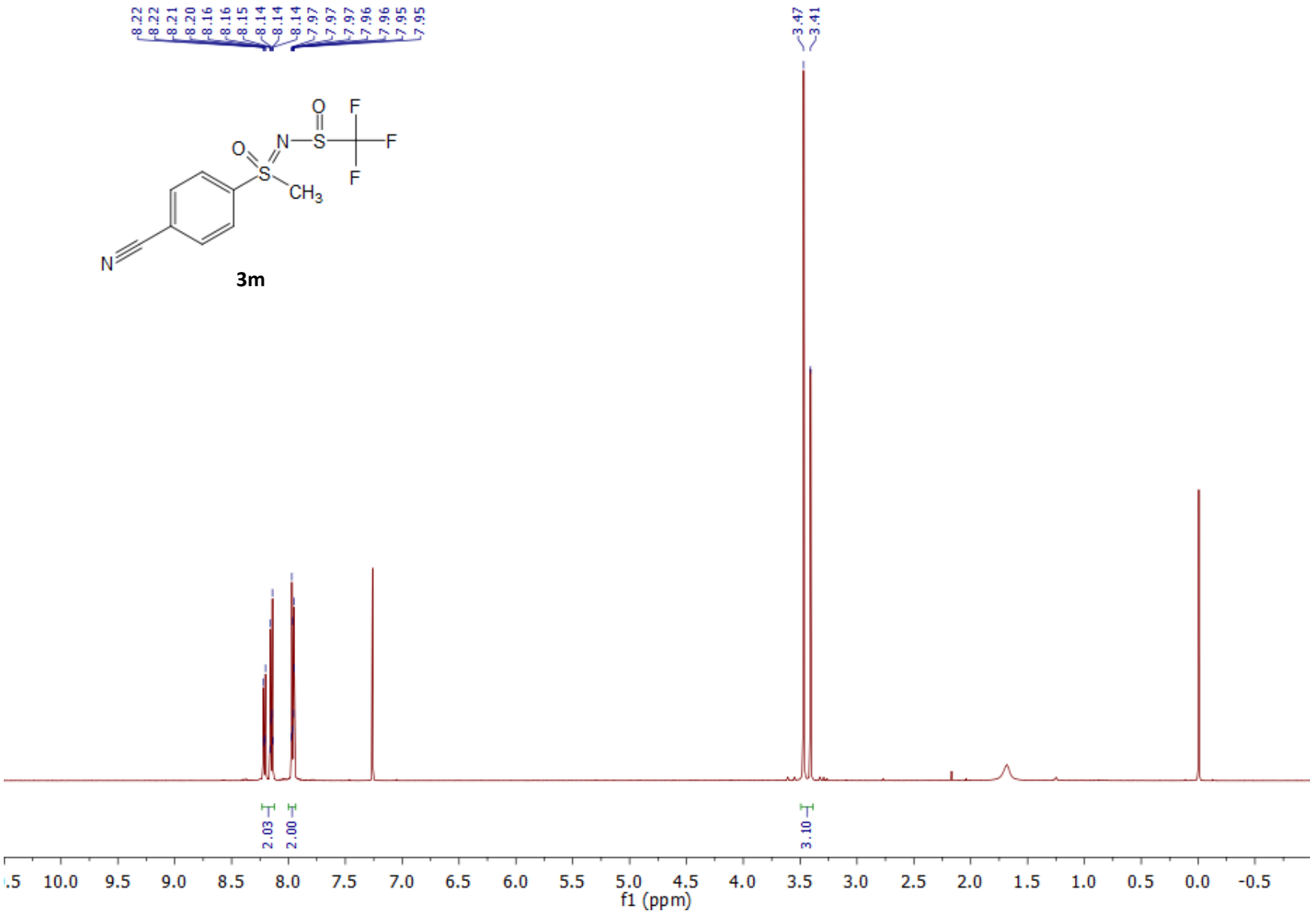

-80.31
-80.56
O
F
O
N
S
F
S
F
CH3
O
N+
O-
3k
80.31
80.56
-79.8
-80.2
-80.6
-81.0
-81.4
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


151.62
151.53
144.27
129.94
129.19
127.96
125.30
125.25
122.64
122.61
119.99
47.45
47.09
O
F
O
N
S
F
S
F
CH3
O
N+
O-
3k
128 127 126 125 124 123 122 121 120 119
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

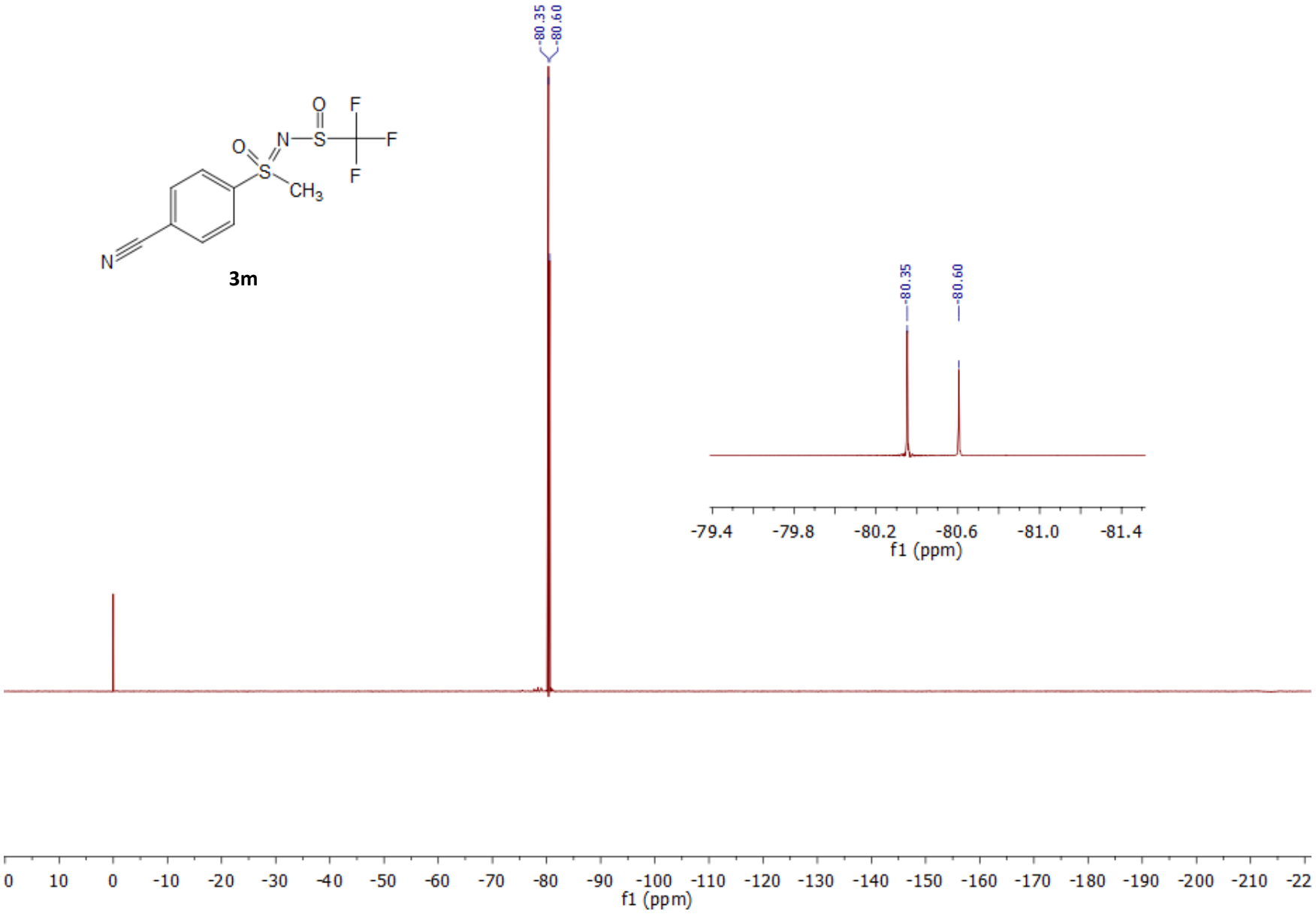

8.33
8.33
8.33
8.30
8.29
8.29
8.28
8.27
8.27
8.27
8.23
8.22
8.22
8.21
8.21
8.21
8.03
8.02
8.01
8.01
7.85
7.84
7.82
3.48
3.42
O
F
O
N
S
F
S
F
CH3
F
F
F
3l
2.13
1.00
1.05
8.3
8.2
8.1
8.0
7.9
7.8
f1 (ppm)
3.13
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

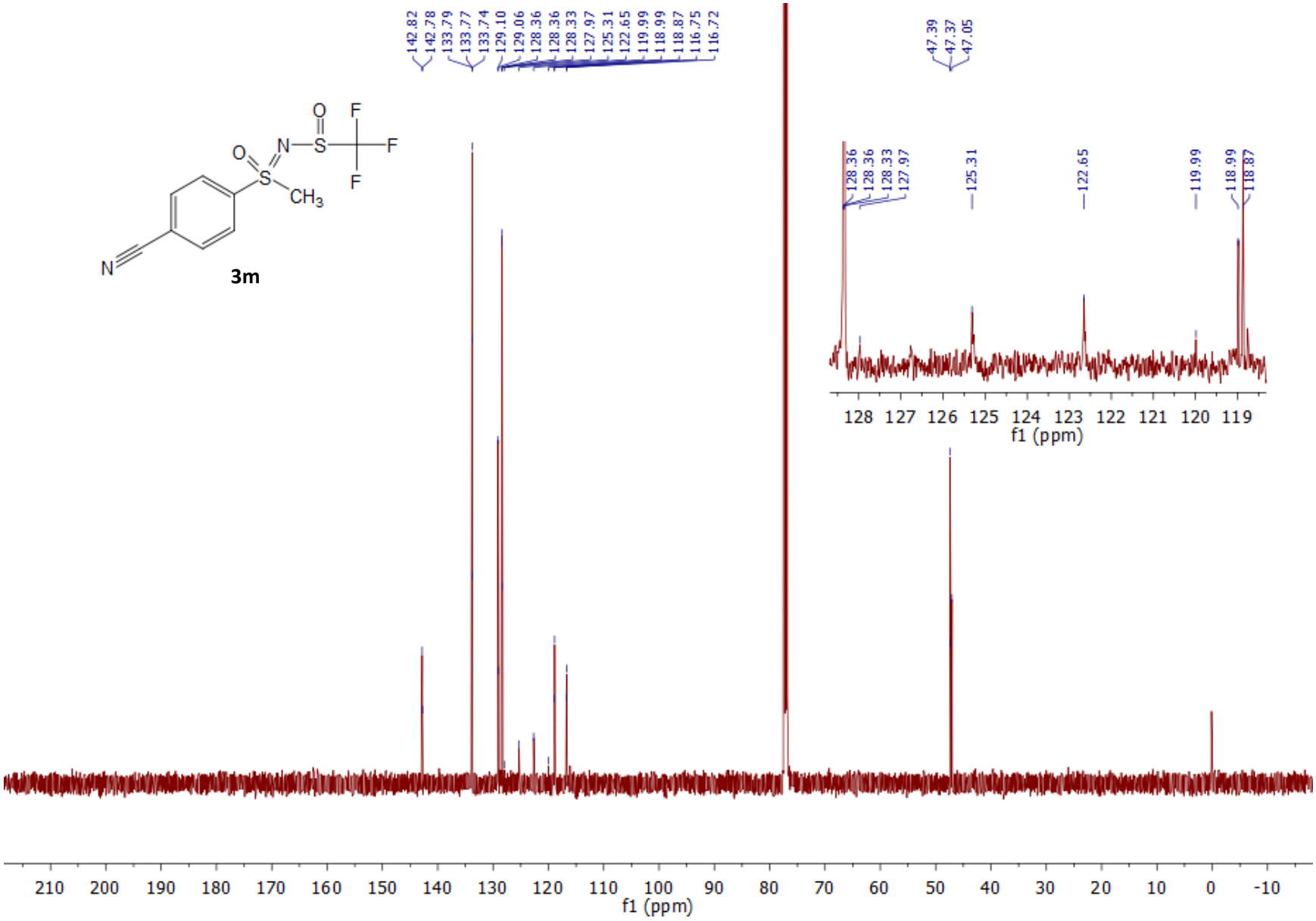

O
F
O
N
S
F
S
F
CH3
F
F
F
3l
-63.39
-63.45
-80.44
-80.65
-62.6 -62.8 -63.0 -63.2 -63.4 -63.6 -63.8 -64.0 -64.2
f1 (ppm)
-79.4 -79.8 -80.2 -80.6 -81.0 -81.4
f1 (ppm)
0 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)

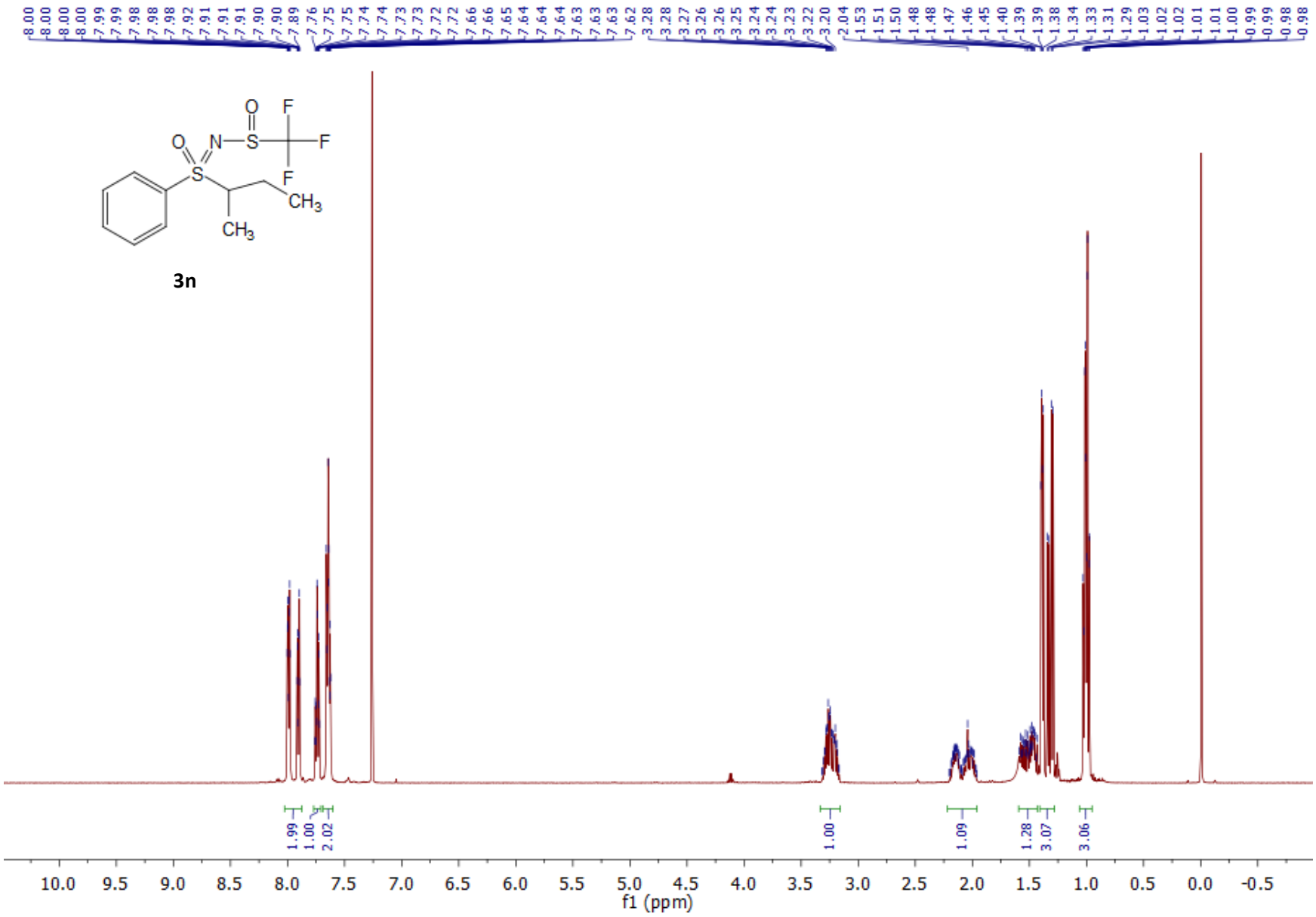

3l
140.02
139.78
133.36
133.09
132.82
132.55
131.90
131.88
131.85
131.74
131.71
131.69
131.66
131.63
131.11
131.05
130.92
128.01
126.14
125.51
125.48
125.35
125.32
124.83
124.80
124.77
124.74
123.96
122.69
122.66
121.79
120.04
119.62
47.53
47.24
f1 (ppm)
f1 (ppm)


8.22
8.22
8.21
8.20
8.16
8.16
8.15
8.14
8.14
8.14
7.97
7.97
7.97
7.96
7.96
7.95
7.95
3.47
3.41
O
F
N
S
F
O
S
F
CH3
N
2.03
2.00
3.10
.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

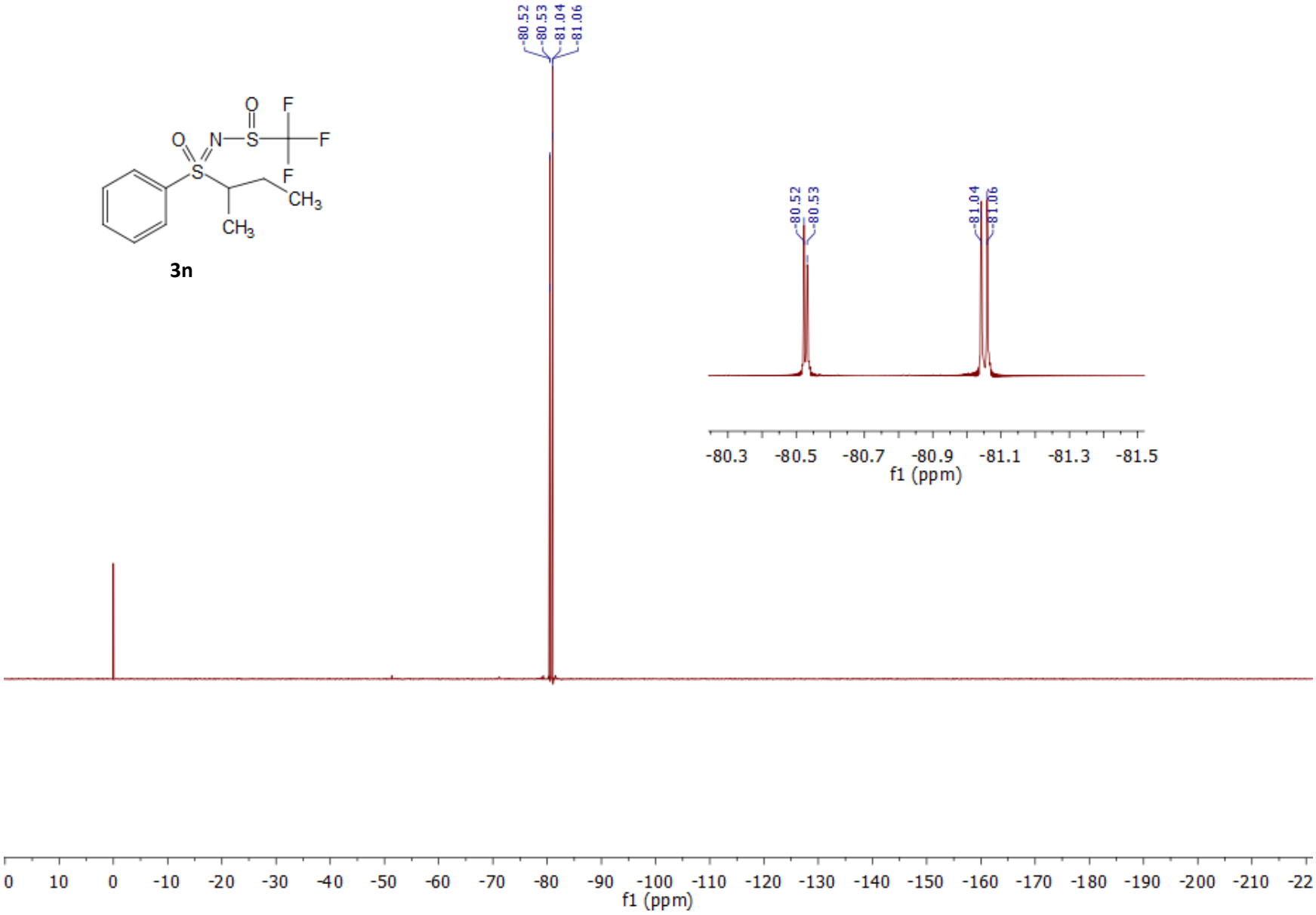
3m


-80.35
-80.60
O
F
N
S
F
O
S
F
CH3
N
3m
-80.35
-80.60
-79.4
-79.8
-80.2
-80.6
-81.0
-81.4
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

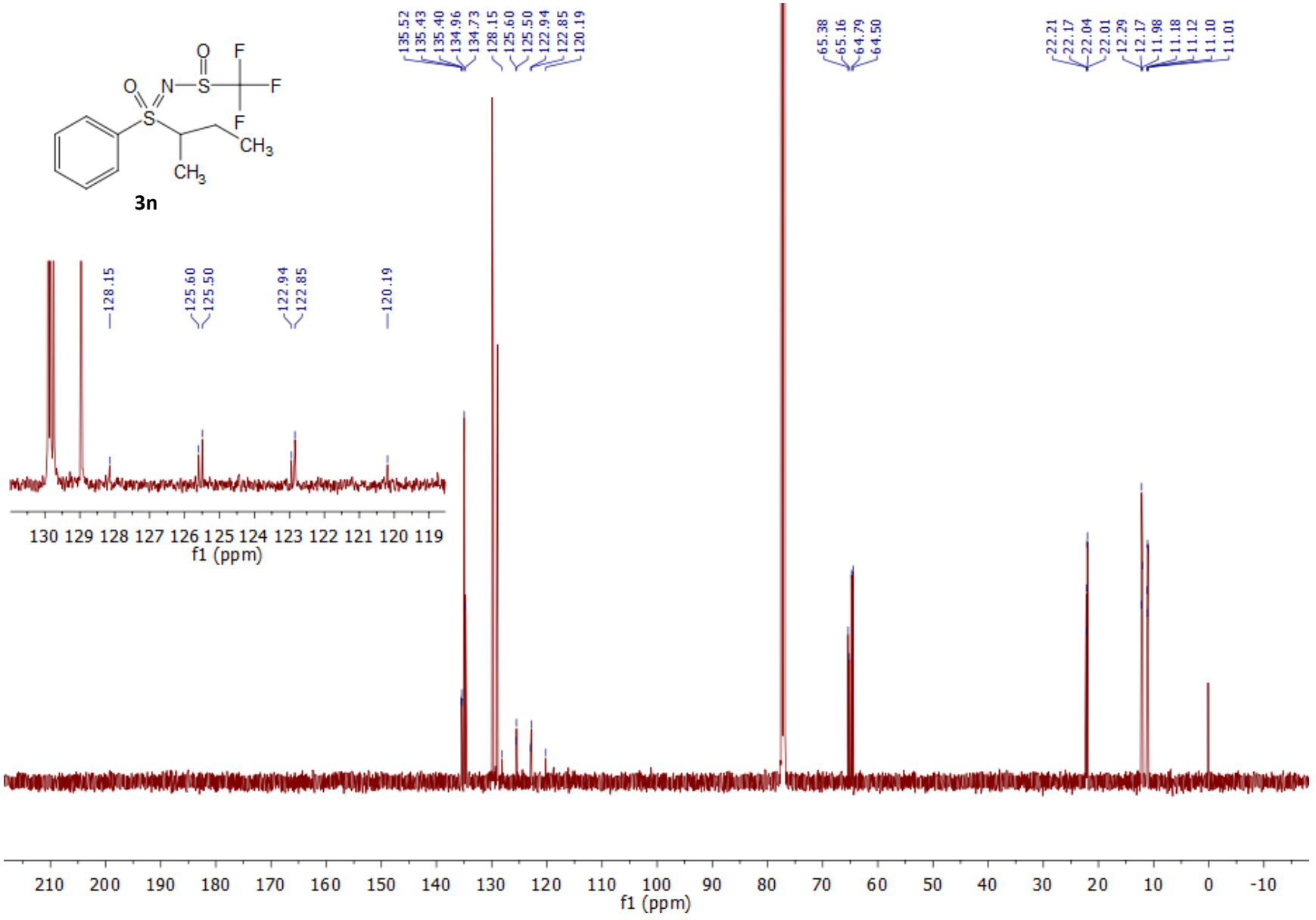

142.82
142.78
133.79
133.77
133.74
129.10
129.06
128.36
128.36
128.33
127.97
125.31
122.65
119.99
118.99
118.87
116.75
116.72
47.39
47.37
47.05
O
F
O
N
S
F
S
F
CH3
N
3m
128.36
128.36
128.33
127.97
125.31
122.65
119.99
118.99
118.87
128 127 126 125 124 123 122 121 120 119
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

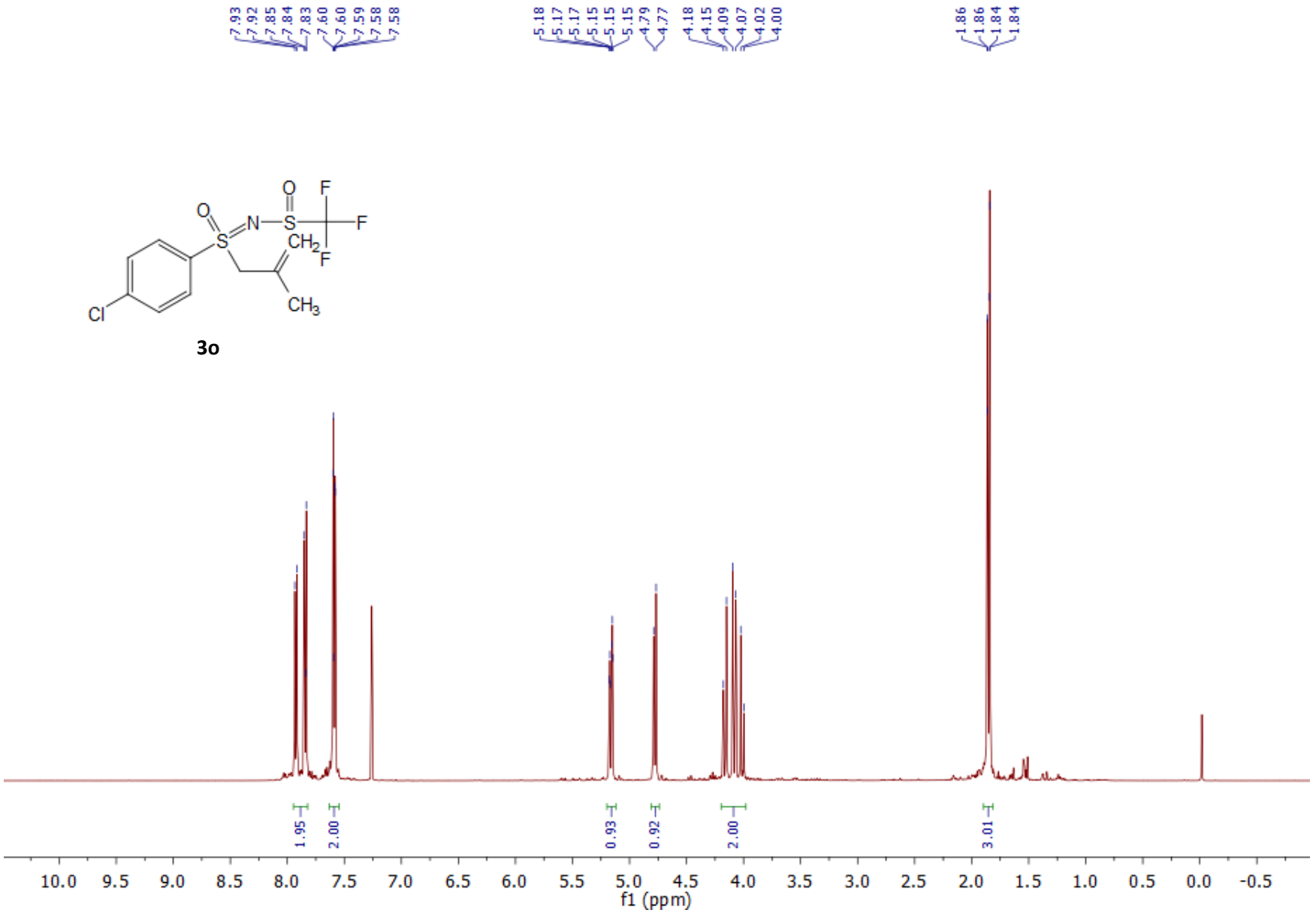

8.00 8.00 8.00 8.00 7.99 7.99 7.99 7.98 7.98 7.98 7.92 7.91 7.91 7.91 7.90 7.90 7.89 7.76 7.75 7.75 7.74 7.74 7.73 7.73 7.72 7.72 7.66 7.66 7.65 7.64 7.64 7.64 7.63 7.63 7.63 7.62 3.28 3.28 3.27 3.26 3.26 3.25 3.24 3.24 3.23 3.22 3.20 2.04 1.53 1.51 1.50 1.48 1.48 1.47 1.46 1.45 1.40 1.39 1.39 1.38 1.34 1.33 1.31 1.29 1.03 1.02 1.02 1.01 1.01 1.00 0.99 0.99 0.98 0.98
O
F
O
N
S
F
S
F
CH3
CH3
1.99
1.00
2.02
1.00
1.09
1.28
3.07
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3n


-80.52
-80.53
-81.04
-81.06
O
F
O
N
S
F
S
F
CH3
CH3
-80.52
-80.53
-81.04
-81.06
-80.3
-80.5
-80.7
-80.9
-81.1
-81.3
-81.5
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

3n

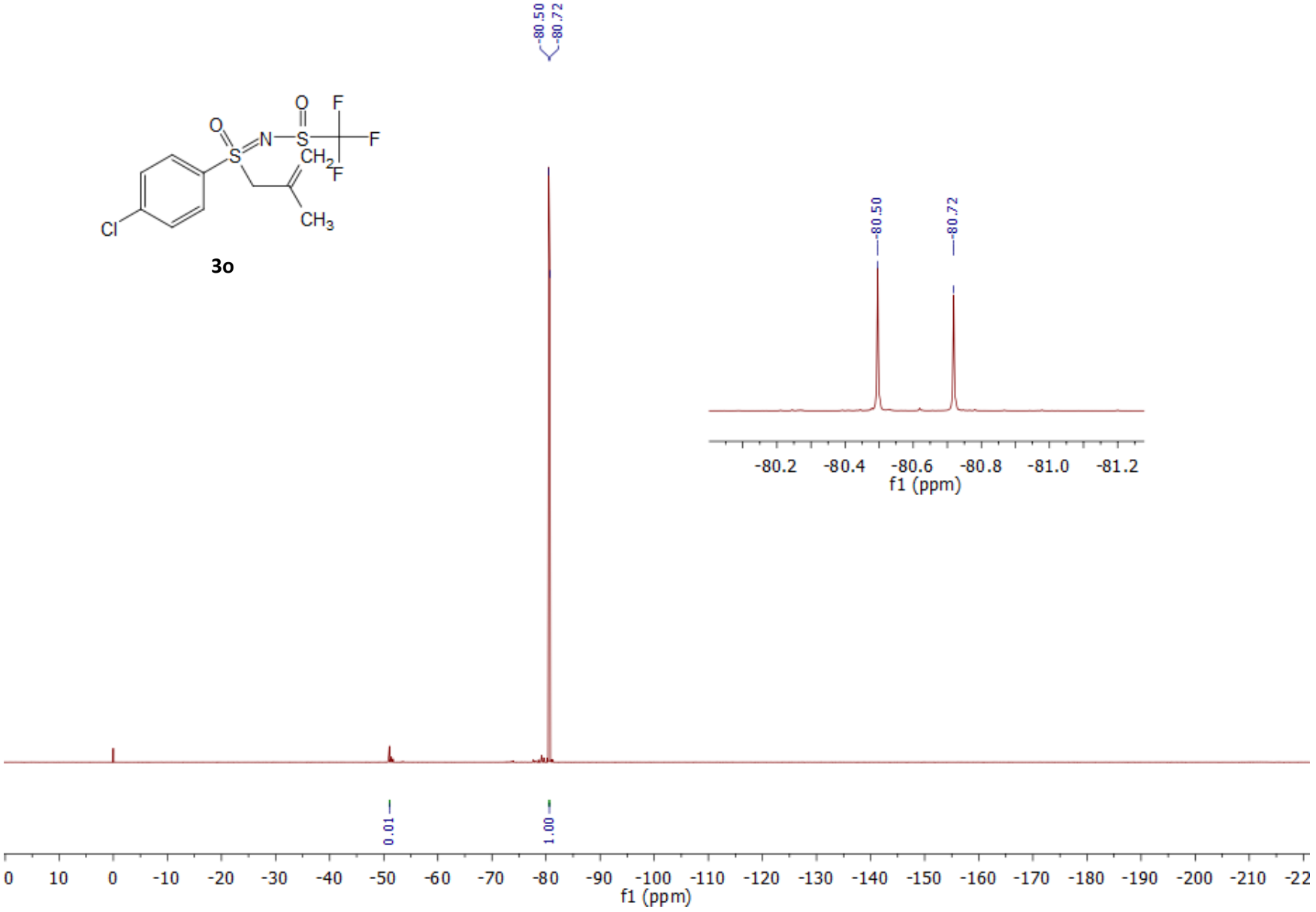

3n
135.52
135.43
135.40
134.96
134.73
128.15
125.60
125.50
122.94
122.85
120.19
65.38
65.16
64.79
64.50
22.21
22.17
22.04
22.01
12.29
12.17
11.98
11.18
11.12
11.10
11.01
130 129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

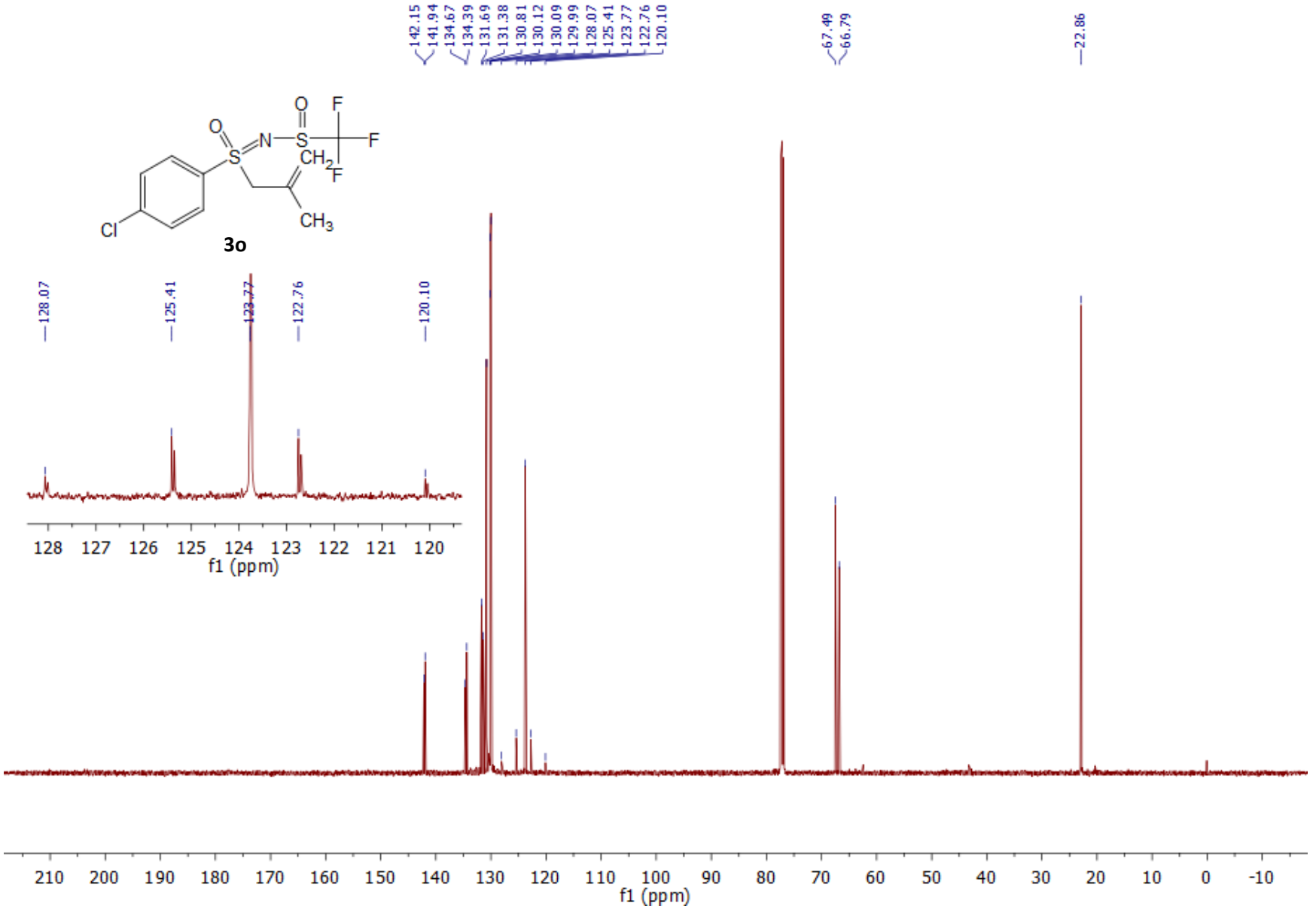

7.93
7.92
7.85
7.84
7.83
7.60
7.60
7.59
7.58
7.58
5.18
5.17
5.17
5.15
5.15
5.15
4.79
4.77
4.18
4.15
4.09
4.07
4.02
4.00
1.86
1.86
1.84
1.84
O
F
O
N
S
F
S
CH2
F
Cl
CH3
1.95
2.00
0.93
0.92
2.00
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

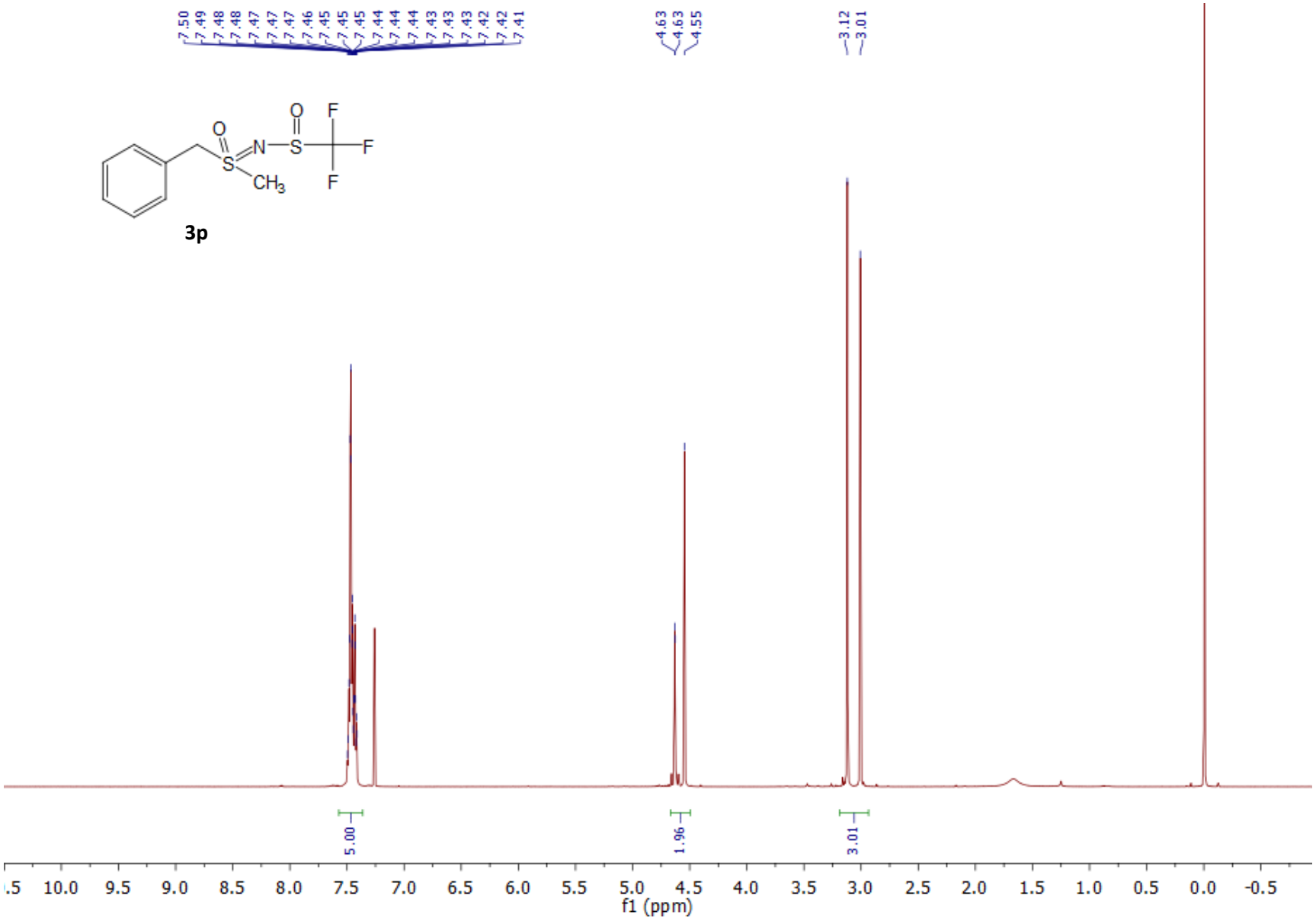
3o

O
F
O
N
S
F
S
CH2
F
Cl
CH3

3o


-80.50
-80.72
-80.50
-80.72
-80.2
-80.4
-80.6
-80.8
-81.0
-81.2
f1 (ppm)
0.01
1.00
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

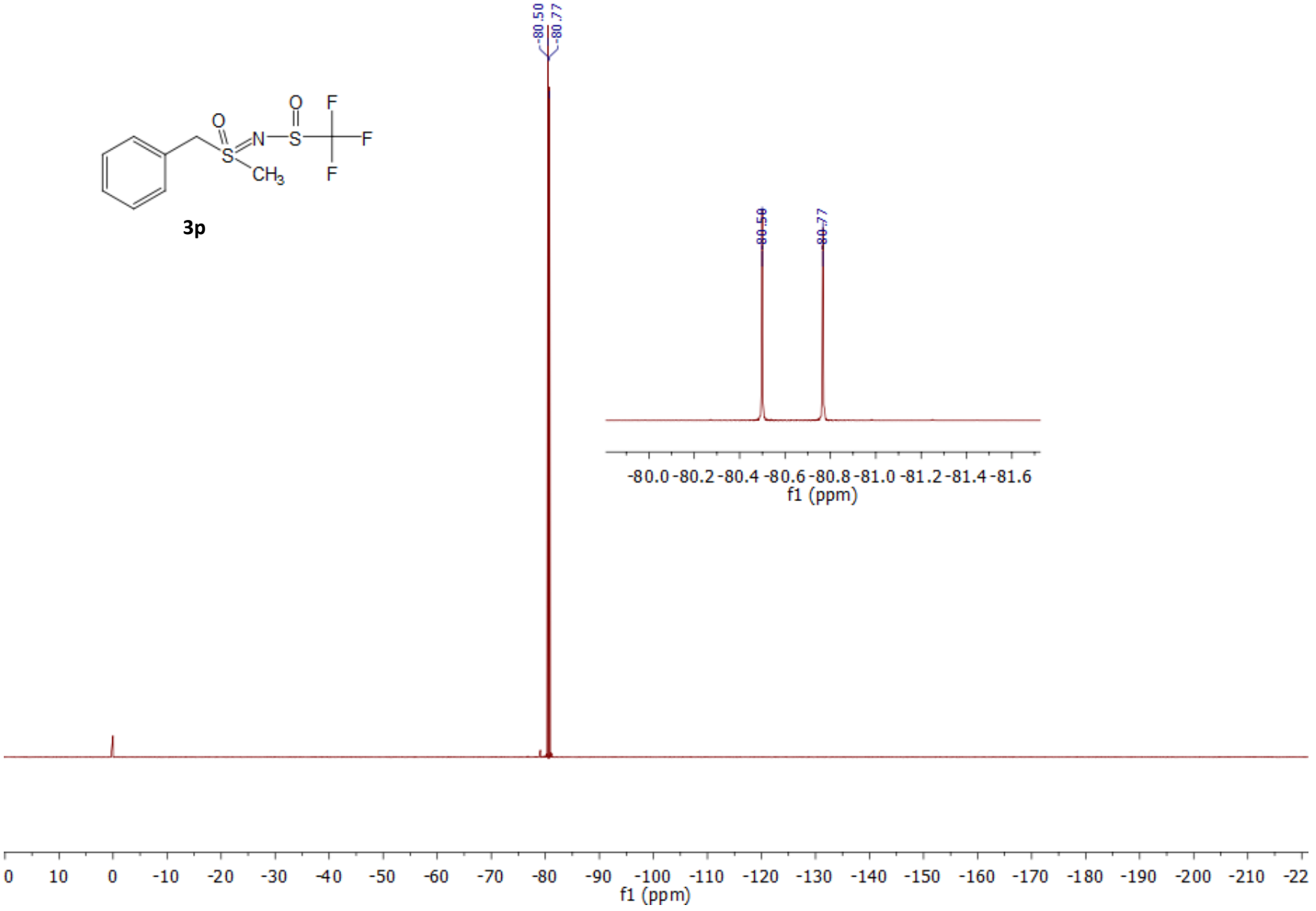

142.15
141.94
134.67
134.39
131.69
131.38
130.81
130.12
130.09
129.99
128.07
125.41
123.77
122.76
120.10
67.49
66.79
22.86
O
O
N
S
S
F
F
CH2
F
Cl
CH3
3o
128.07
125.41
123.77
122.76
120.10
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

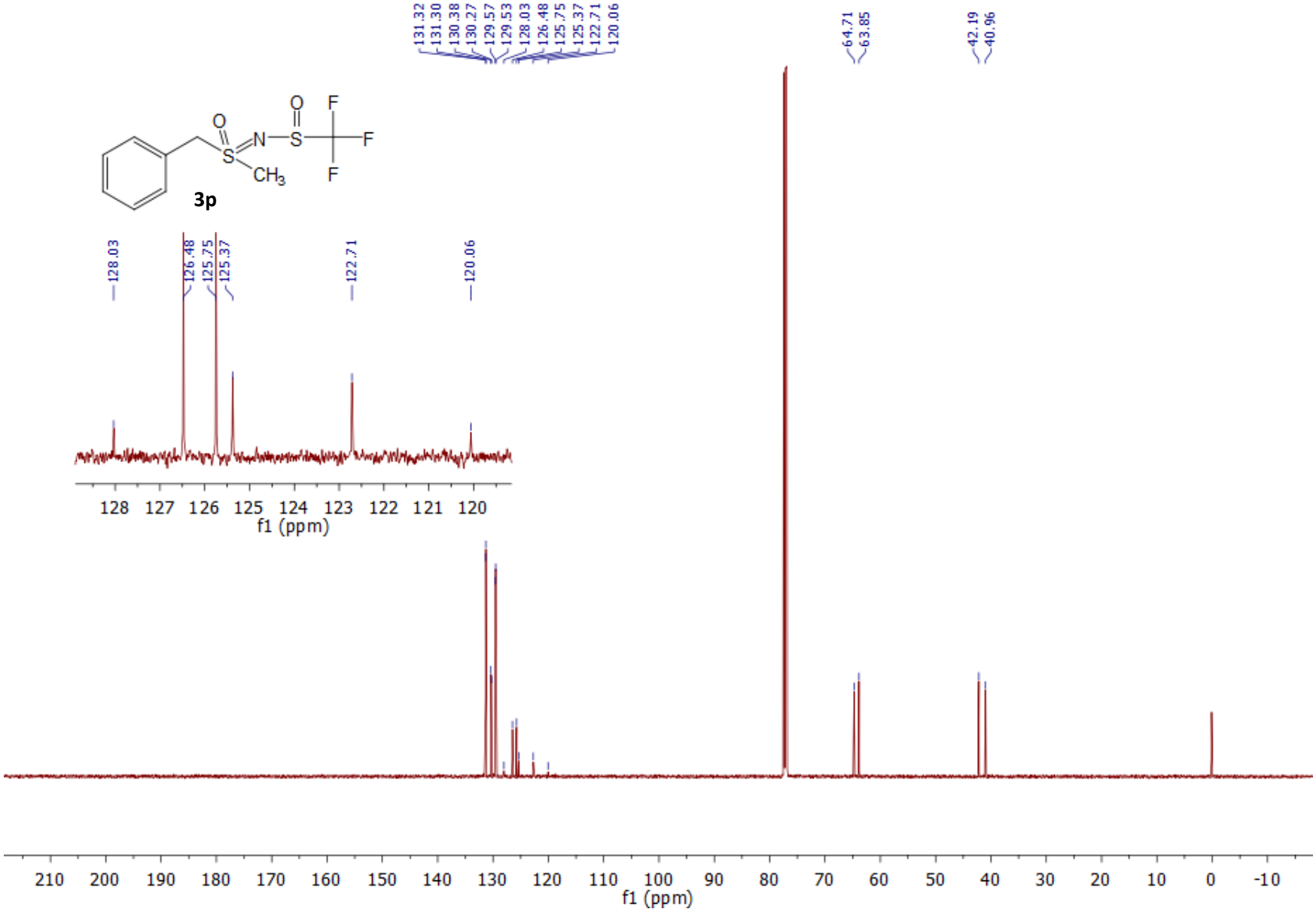

7.50
7.49
7.48
7.48
7.47
7.47
7.47
7.46
7.45
7.45
7.45
7.44
7.44
7.44
7.43
7.43
7.43
7.42
7.42
7.41
4.63
4.63
4.55
3.12
3.01
O
F
O
N
S
F
S
CH3
F
5.00
1.96
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

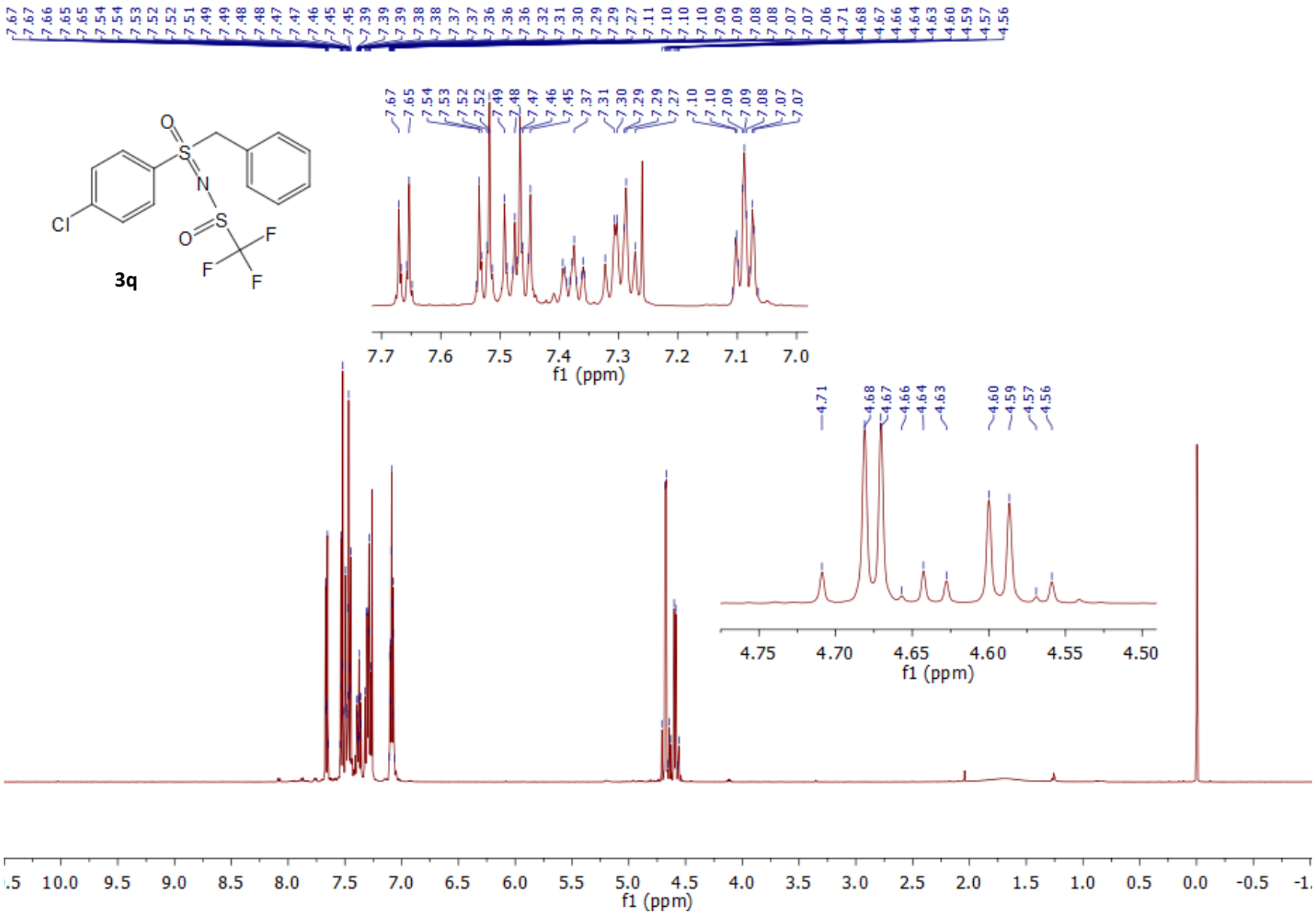
3p

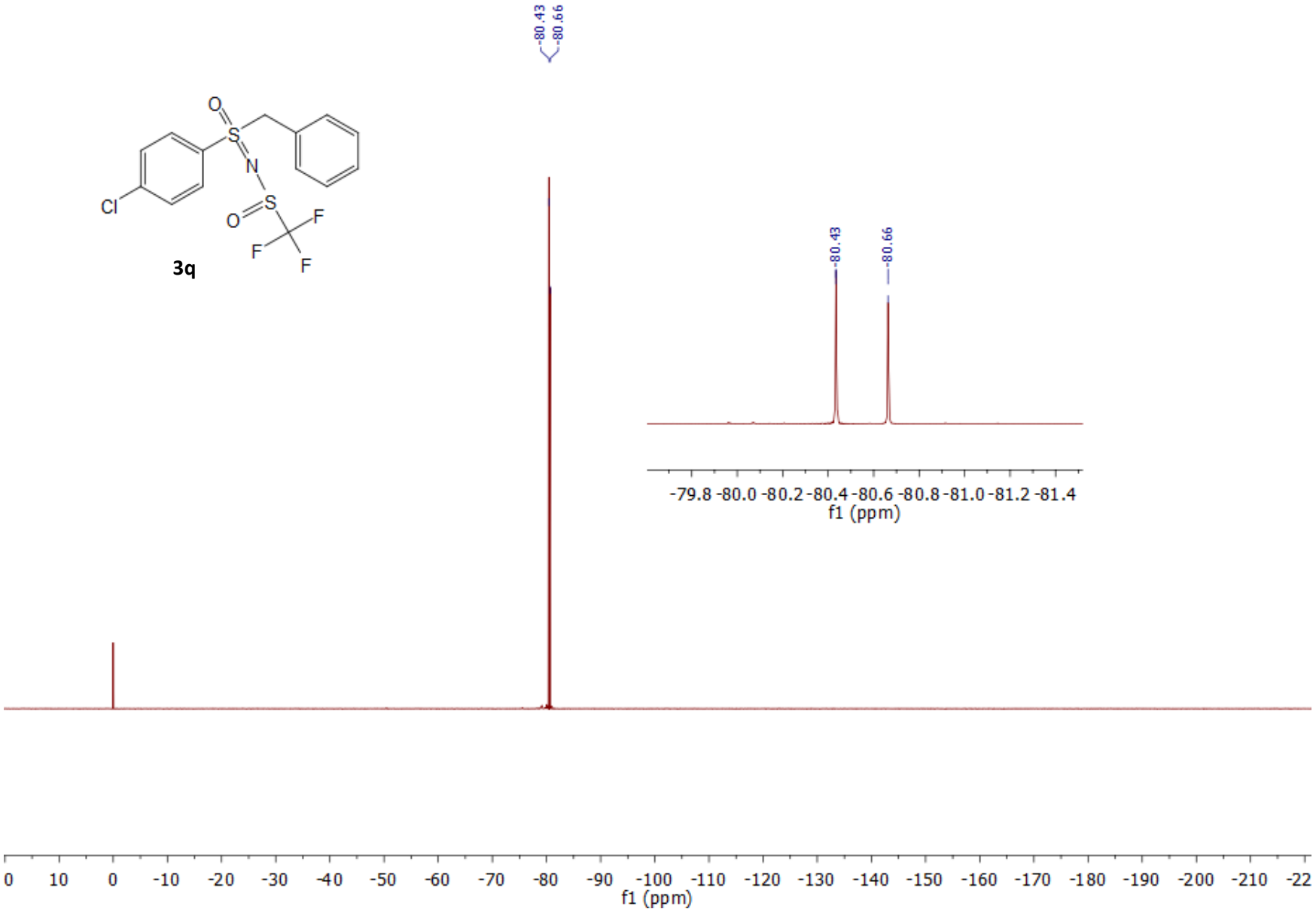
O
F
O
N
S
F
S
CH3
F

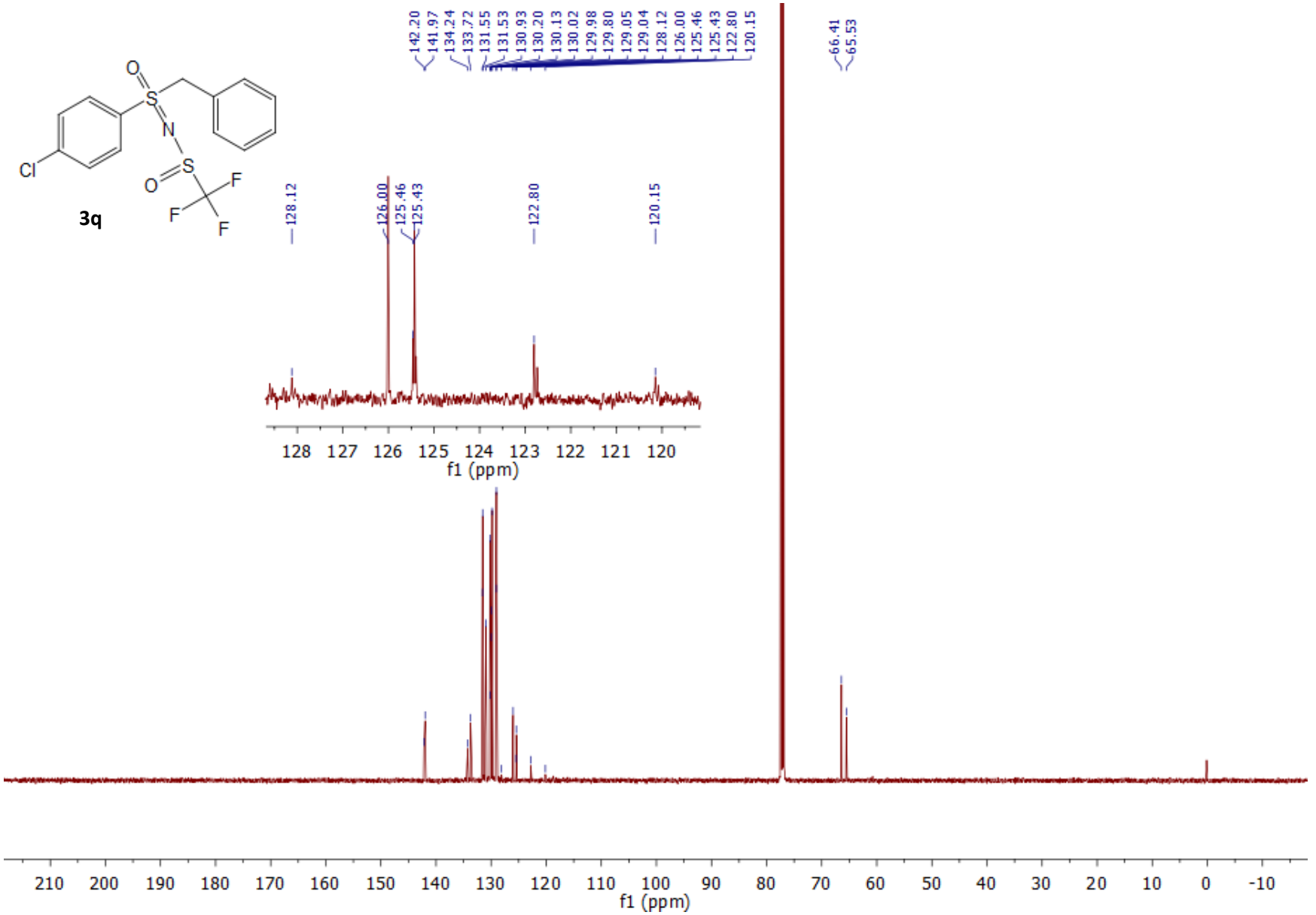
3p

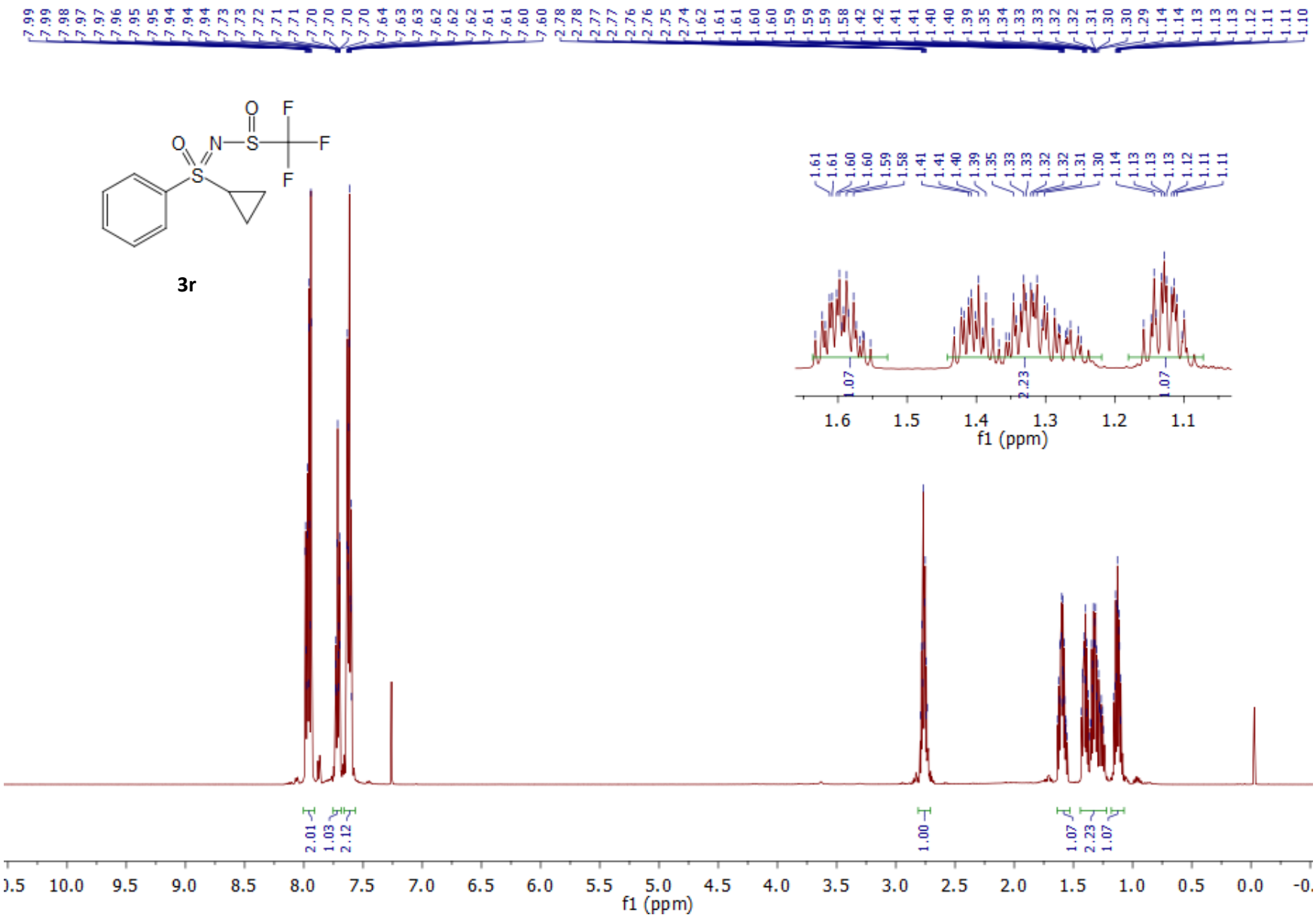

-80.50
-80.77
-80.50
-80.77
-80.0 -80.2 -80.4 -80.6 -80.8 -81.0 -81.2 -81.4 -81.6
f1 (ppm)
0 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)

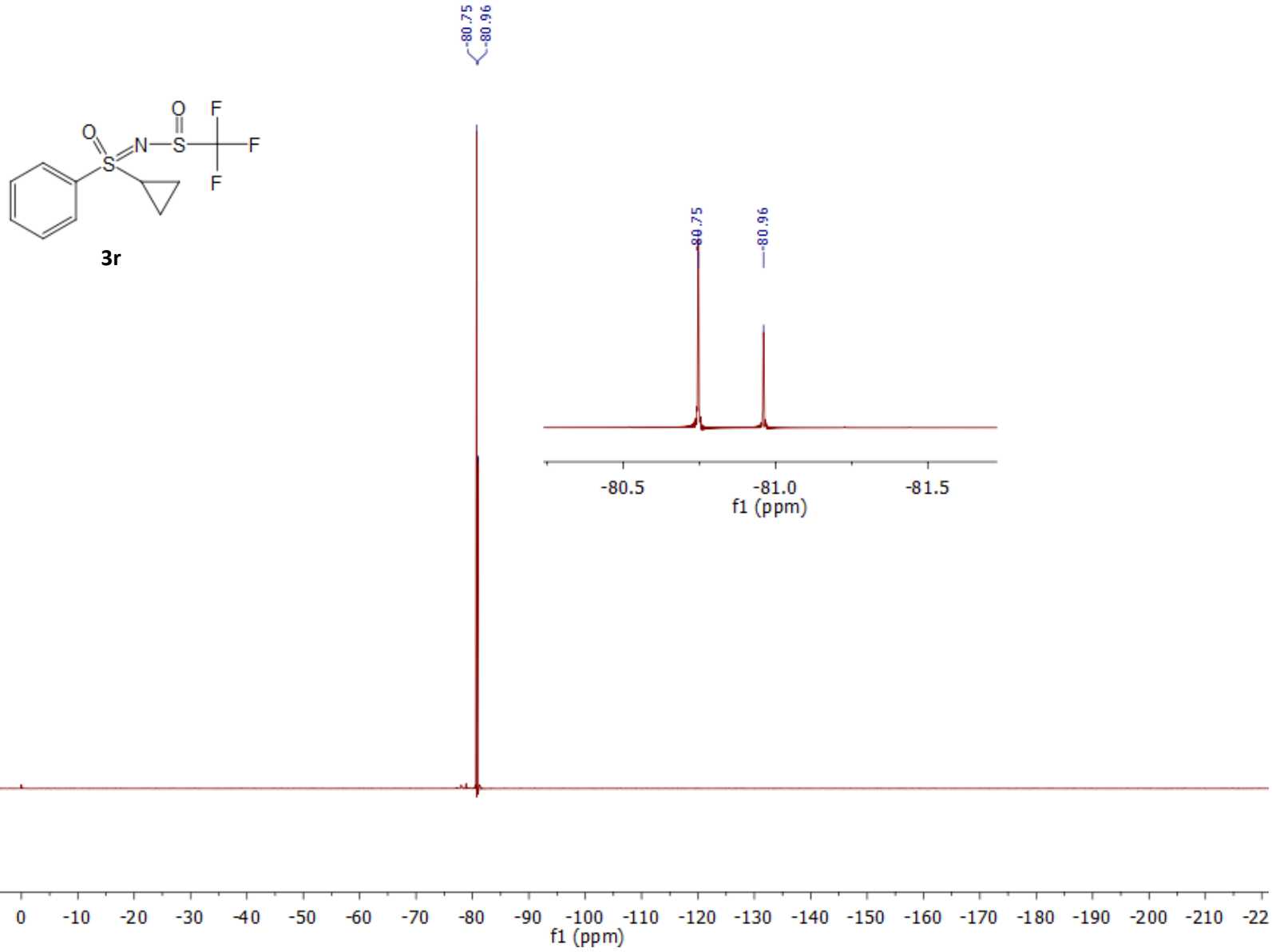

131.32
131.30
130.38
130.27
129.57
129.53
128.03
126.48
125.75
125.37
122.71
120.06
64.71
63.85
42.19
40.96
O
F
O
N
S
F
S
CH3
F
3p
128.03
126.48
125.75
125.37
122.71
120.06
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

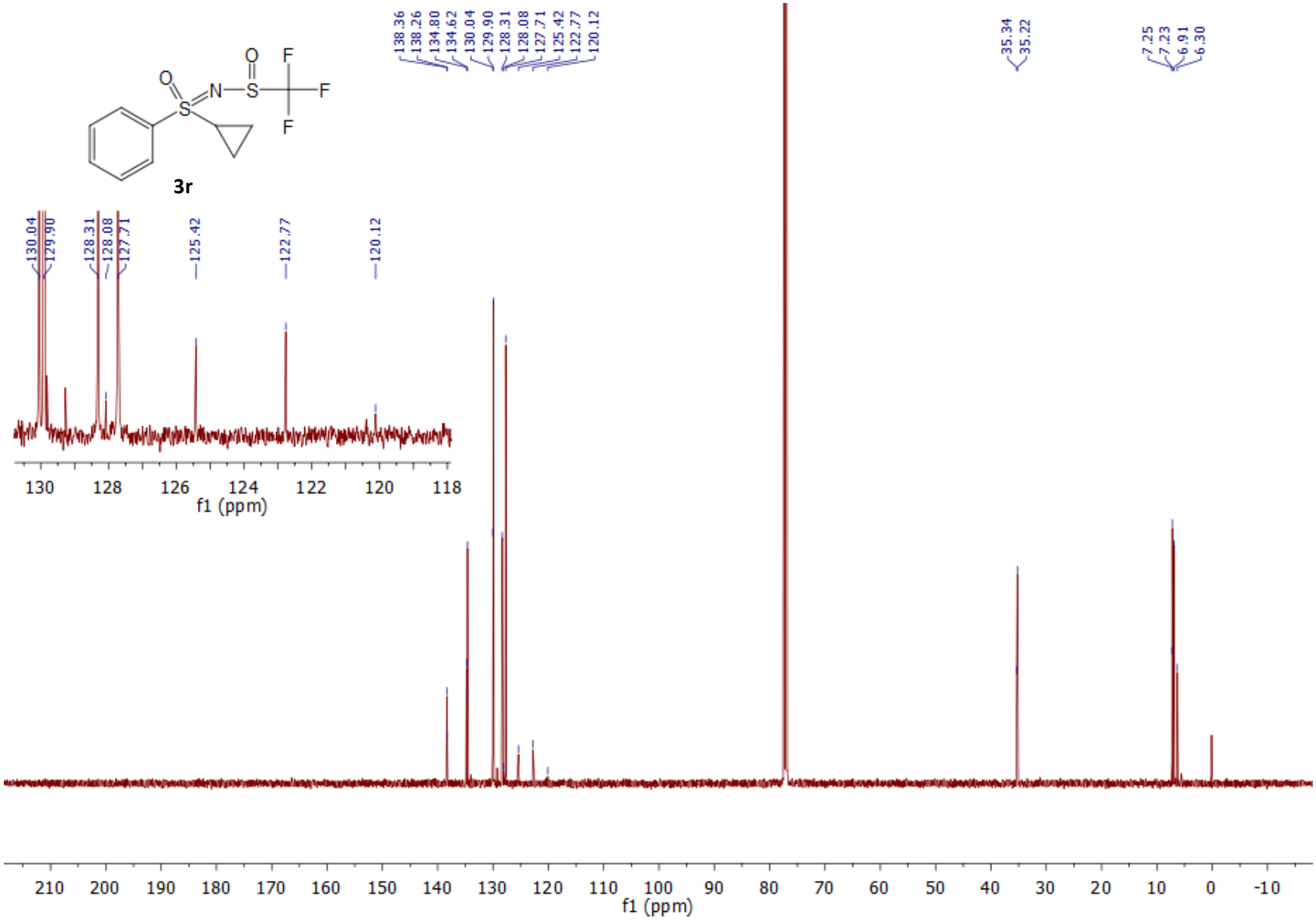

7.67 7.67 7.66 7.65 7.65 7.54 7.54 7.53 7.52 7.52 7.51 7.49 7.49 7.48 7.48 7.47 7.47 7.46 7.45 7.45 7.39 7.39 7.39 7.38 7.38 7.37 7.37 7.36 7.36 7.36 7.32 7.31 7.30 7.29 7.29 7.27 7.11 7.10 7.10 7.10 7.09 7.09 7.08 7.08 7.07 7.07 7.06 4.71 4.68 4.67 4.66 4.64 4.63 4.60 4.59 4.57 4.56
Cl
O
S
N
S
O
F
F
F
3q
7.67 7.65 7.54 7.53 7.52 7.52 7.49 7.48 7.47 7.46 7.45 7.37 7.31 7.30 7.29 7.29 7.27 7.10 7.10 7.09 7.09 7.08 7.07 7.07
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
4.71 4.68 4.67 4.66 4.64 4.63 4.60 4.59 4.57 4.56
4.75 4.70 4.65 4.60 4.55 4.50
f1 (ppm)
.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

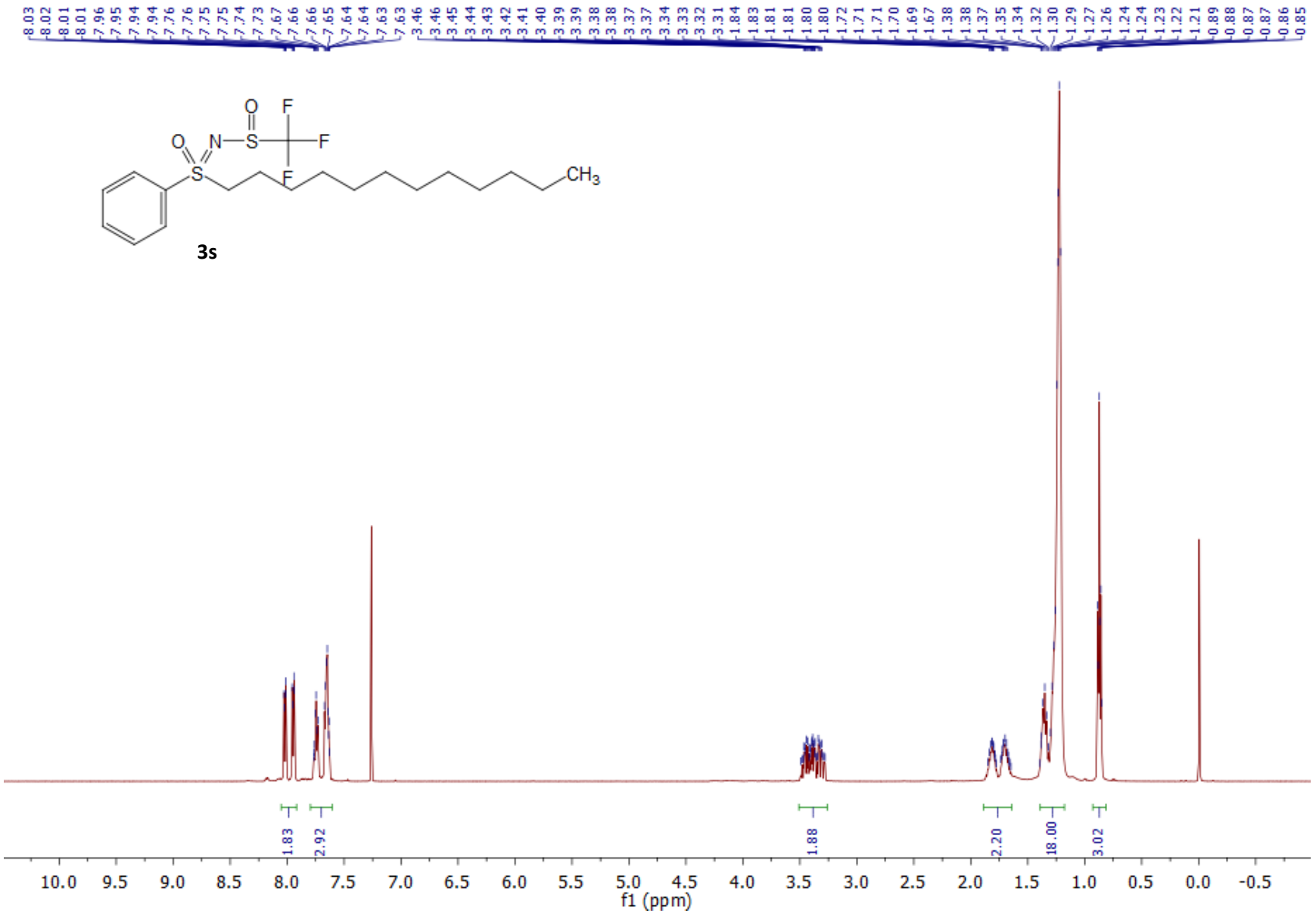

-80.43
-80.66
O
S
N
S
O
F
F
F
Cl
3q
-80.43
-80.66
-79.8 -80.0 -80.2 -80.4 -80.6 -80.8 -81.0 -81.2 -81.4
f1 (ppm)
0 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)


142.20
141.97
134.24
133.72
131.55
131.53
130.93
130.20
130.13
130.02
129.98
129.80
129.05
129.04
128.12
126.00
125.46
125.43
122.80
120.15
66.41
65.53
Cl
O
S
N
S
O
F
F
F
3q
128.12
126.00
125.46
125.43
122.80
120.15
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

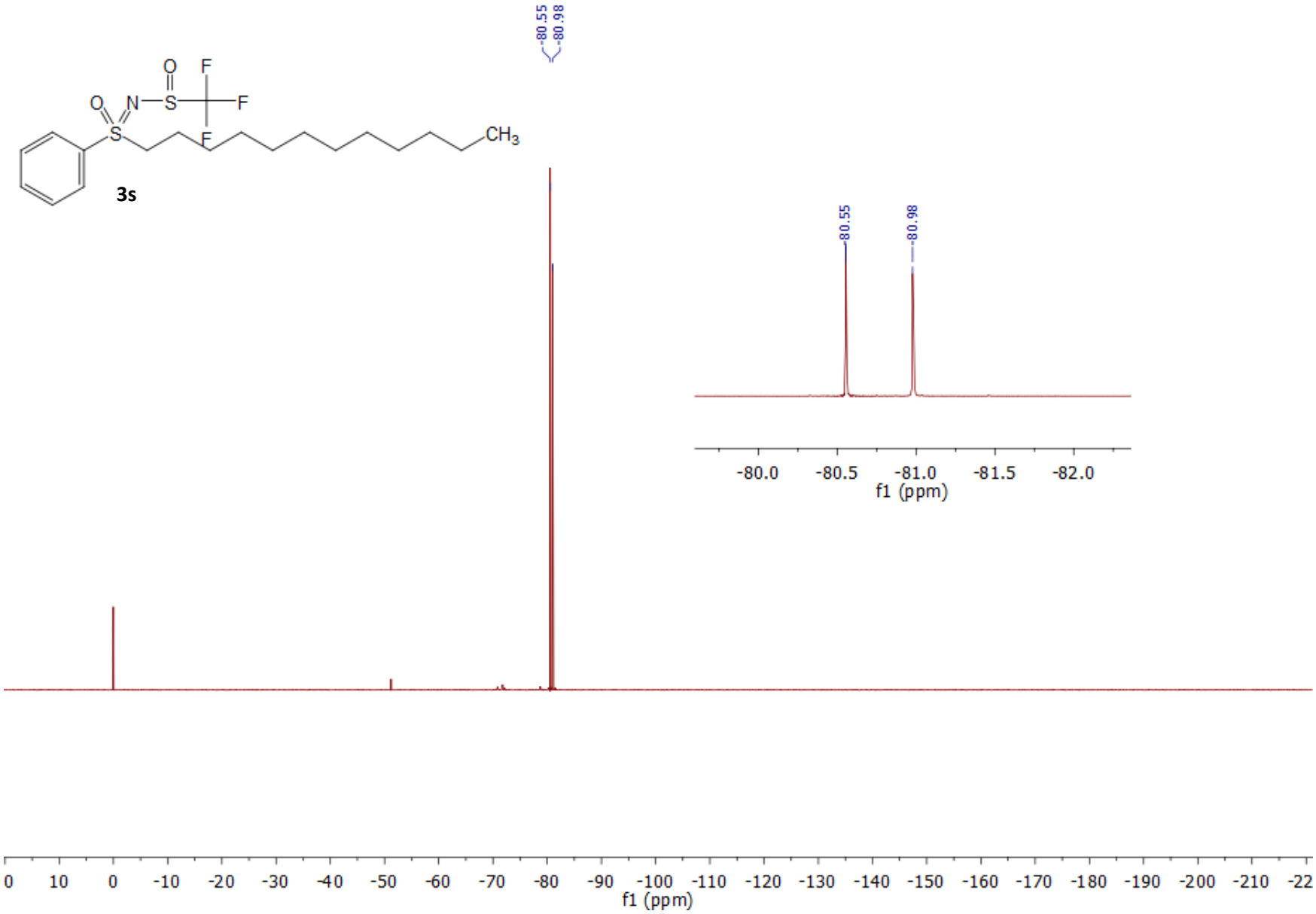

3r
f1 (ppm)

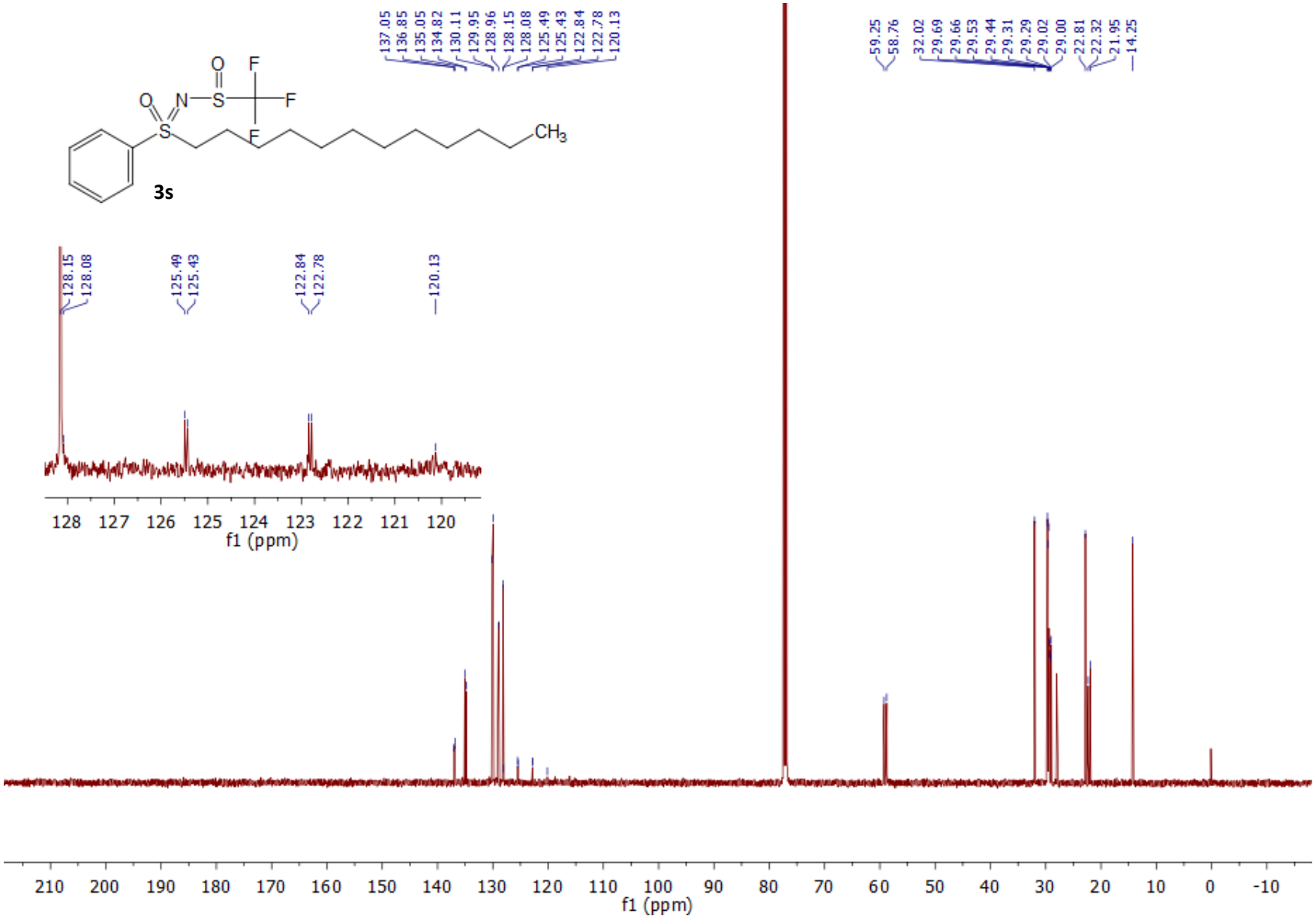

-80.75
-80.96
O
F
O
N
S
F
S
F
3r
-80.75
-80.96
-80.5
-81.0
-81.5
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

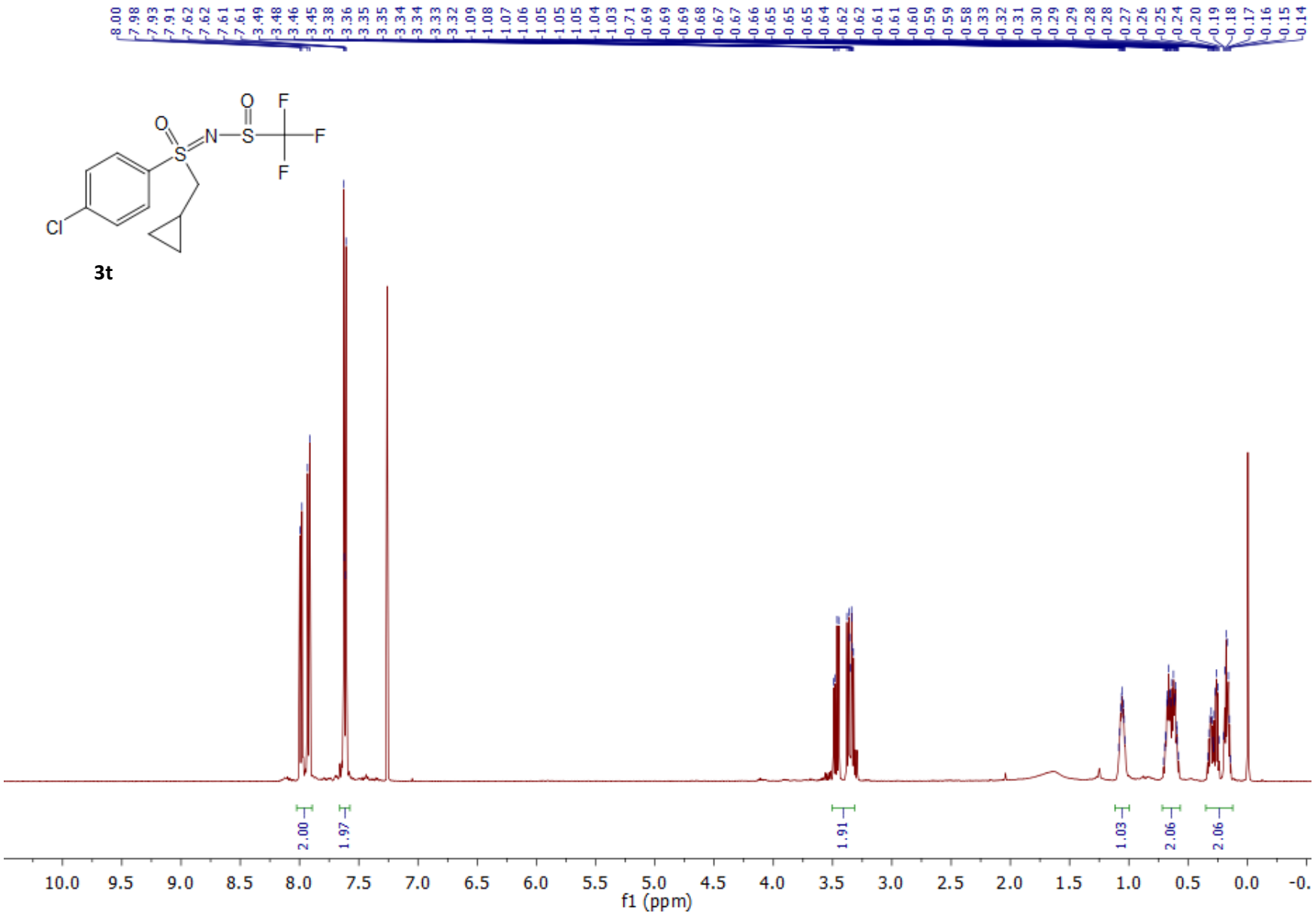

138.36
138.26
134.80
134.62
130.04
129.90
128.31
128.08
127.71
125.42
122.77
120.12
35.34
35.22
7.25
7.23
6.91
6.30
O
O
N
S
S
F
F
F
3r
f1 (ppm)
f1 (ppm)


8.03 8.02 8.01 8.01 7.96 7.95 7.94 7.94 7.76 7.76 7.75 7.75 7.74 7.73 7.67 7.66 7.66 7.65 7.64 7.64 7.63 7.63
3.46 3.46 3.45 3.44 3.43 3.42 3.41 3.40 3.39 3.39 3.38 3.38 3.37 3.37 3.34 3.33 3.32 3.31 1.84 1.83 1.81 1.81 1.80 1.80 1.72 1.71 1.71 1.70 1.69 1.67 1.38 1.38 1.37 1.35 1.34 1.32 1.30 1.29 1.27 1.26 1.24 1.24 1.23 1.22 1.21 0.89 0.88 0.87 0.87 0.86 0.85
O F O N S F F S CH3
1.83 2.92 1.88 2.20 18.00 3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

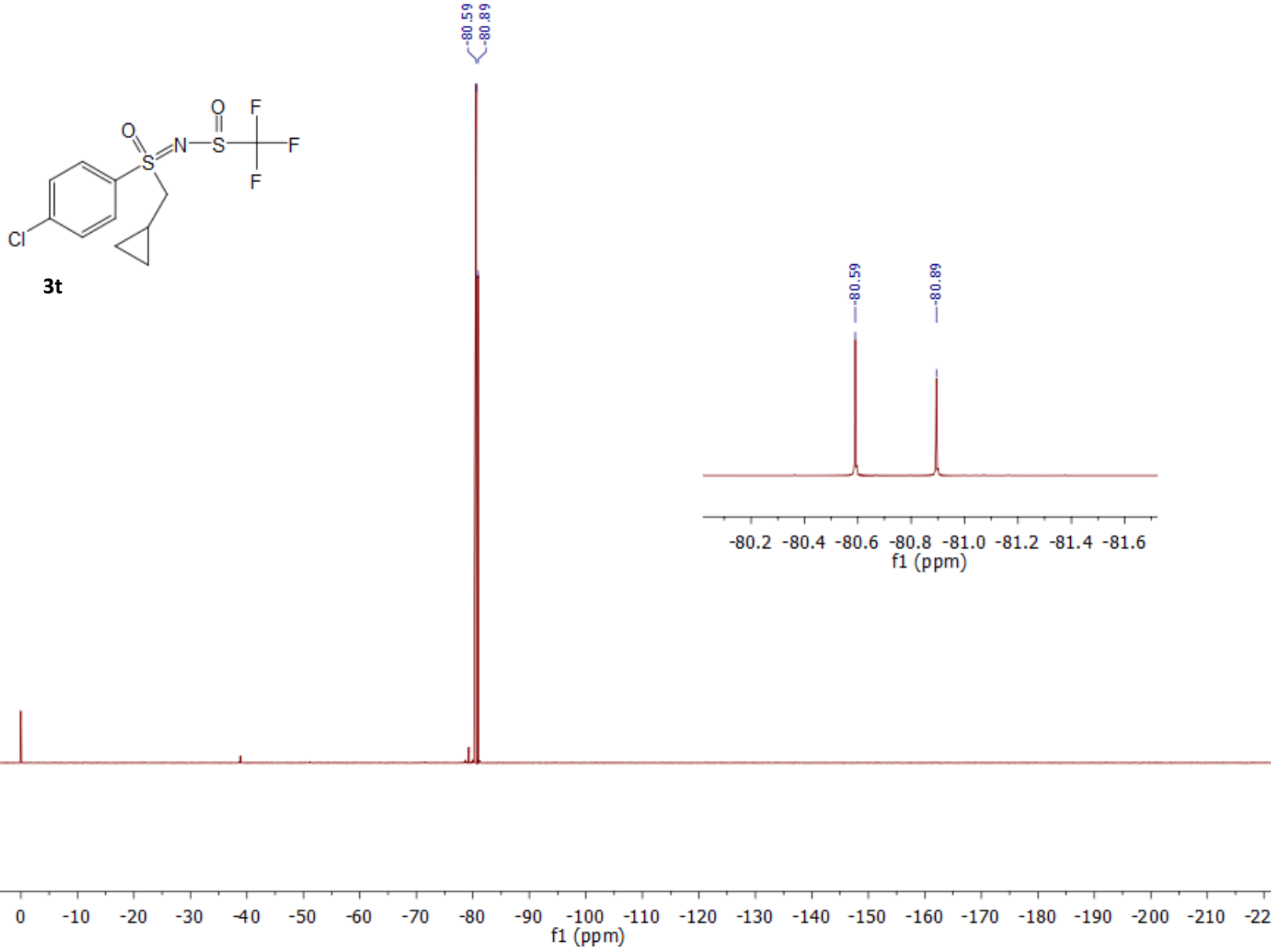
3s

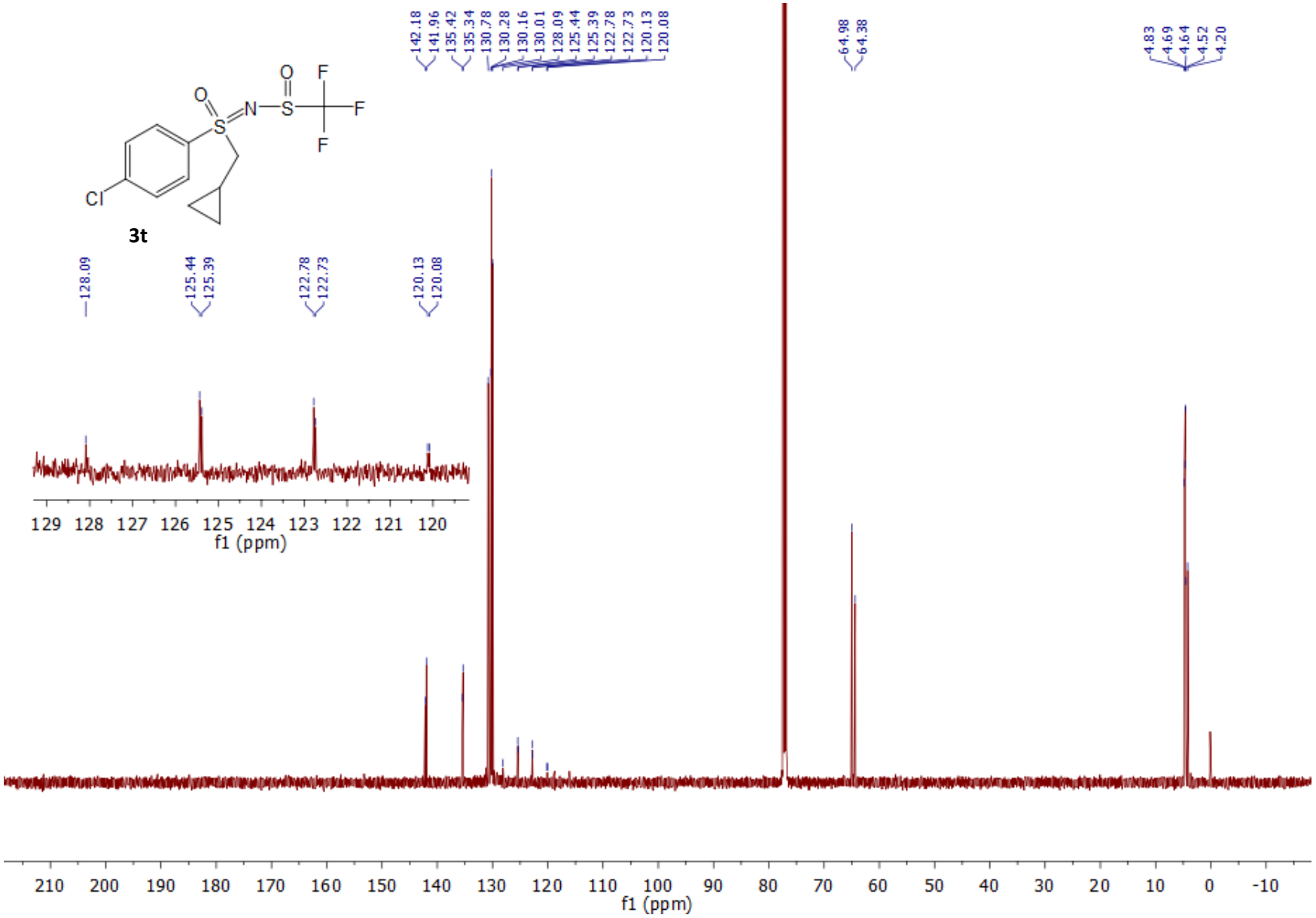

-80.55
-80.98
O
F
O
N
S
F
S
F
CH3
3s
-80.55
-80.98
-80.0
-80.5
-81.0
-81.5
-82.0
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

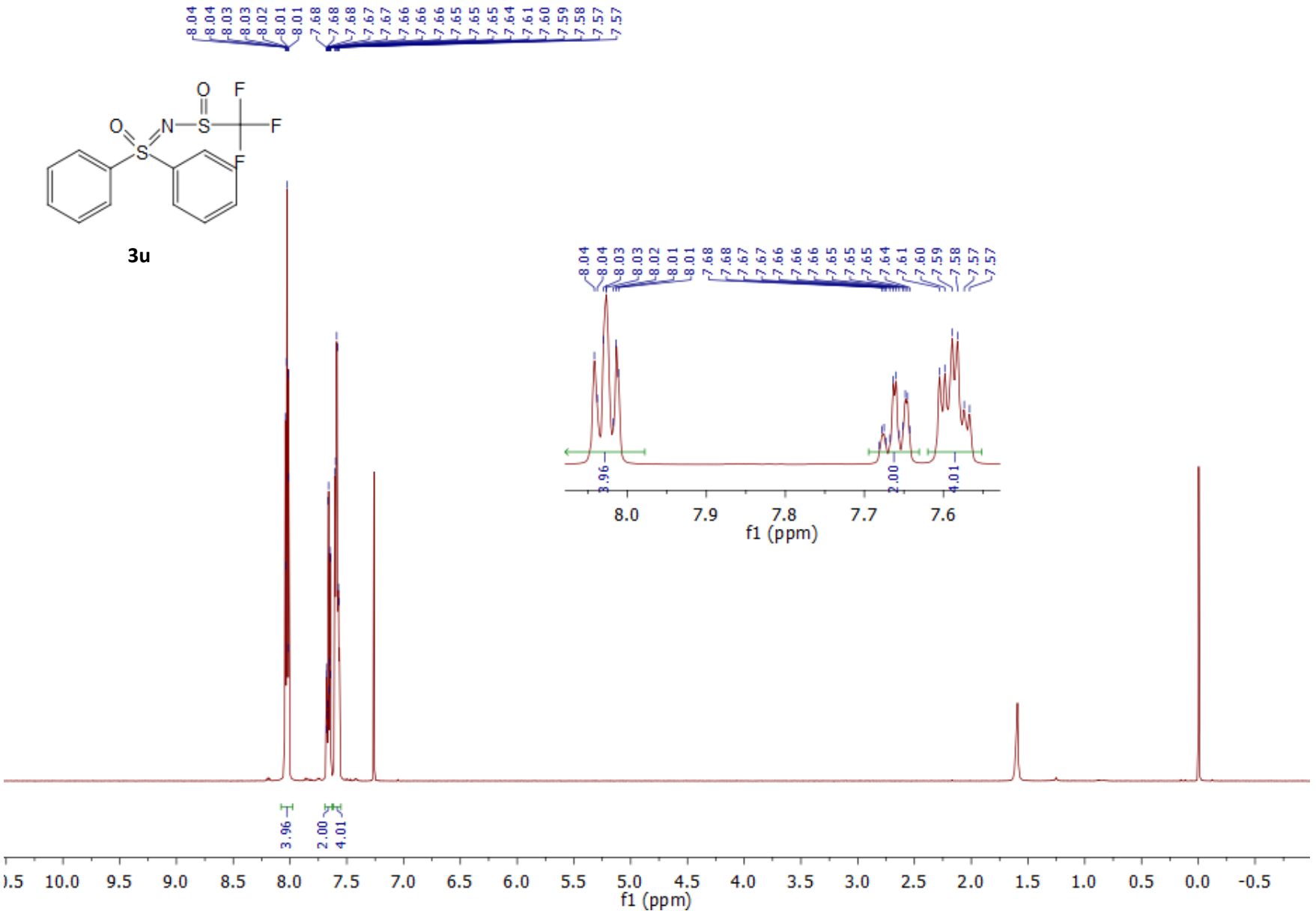

137.05
136.85
135.05
134.82
130.11
129.95
128.96
128.15
128.08
125.49
125.43
122.84
122.78
120.13
59.25
58.76
32.02
29.69
29.66
29.53
29.44
29.31
29.29
29.02
29.00
22.81
22.32
21.95
14.25
O
F
O
N
S
F
S
F
CH3
3s
128.15
128.08
125.49
125.43
122.84
122.78
120.13
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.00 7.98 7.93 7.91 7.62 7.62 7.61 7.61 3.49 3.48 3.46 3.45 3.38 3.36 3.35 3.35 3.34 3.34 3.33 3.32 1.09 1.08 1.07 1.06 1.05 1.05 1.05 1.04 1.03 0.71 0.69 0.69 0.69 0.68 0.67 0.67 0.66 0.65 0.65 0.65 0.64 0.62 0.62 0.61 0.61 0.60 0.59 0.59 0.58 0.33 0.32 0.31 0.30 0.29 0.29 0.28 0.28 0.27 0.26 0.25 0.24 0.20 0.19 0.18 0.17 0.16 0.15 0.14
O
F
O
N
S
S
F
F
Cl
2.00
1.97
1.91
1.03
2.06
2.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

3t

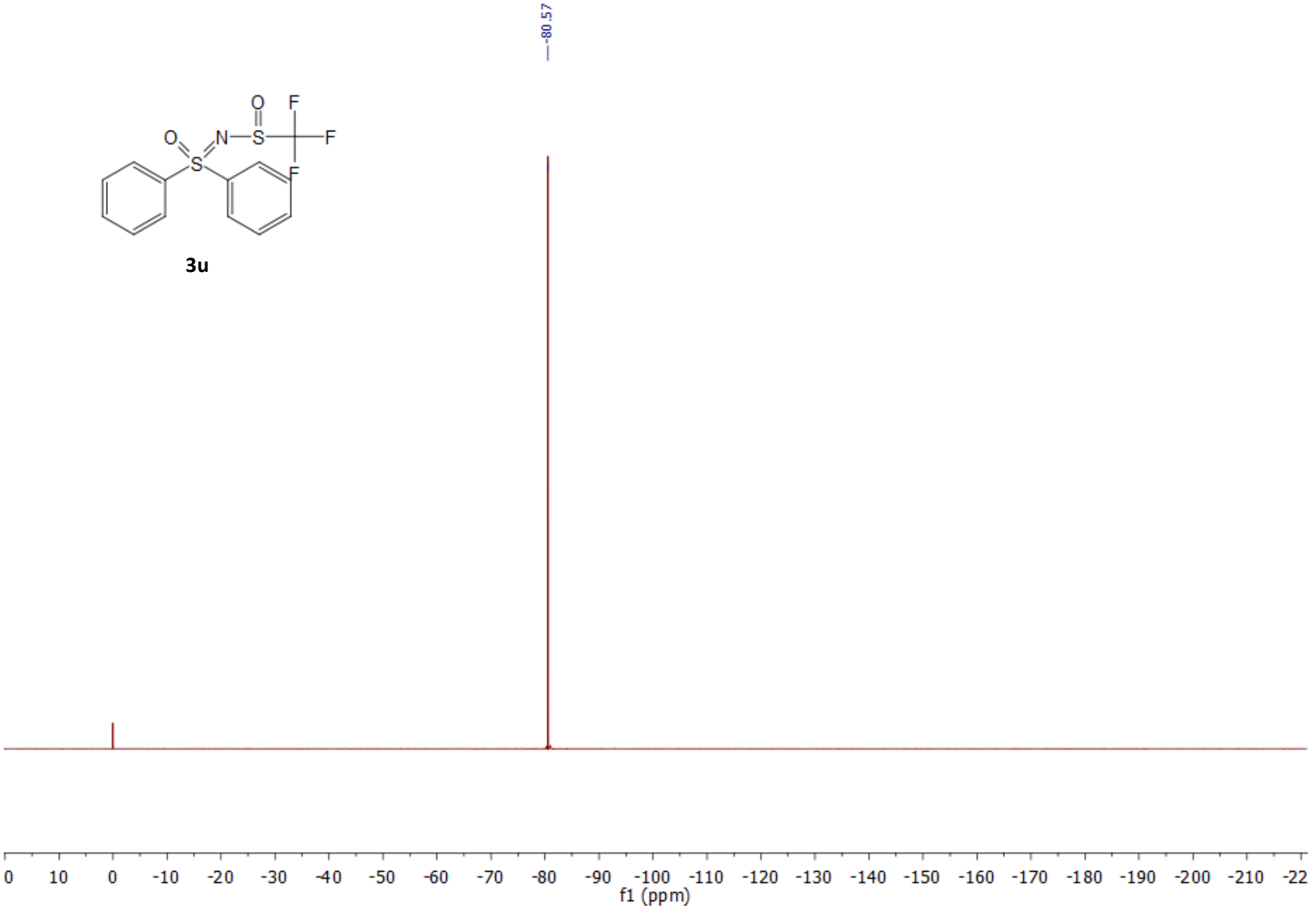

-80.59
-80.89
O
F
O
N
S
F
S
F
Cl
3t
-80.59
-80.89
-80.2 -80.4 -80.6 -80.8 -81.0 -81.2 -81.4 -81.6
f1 (ppm)
0 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)

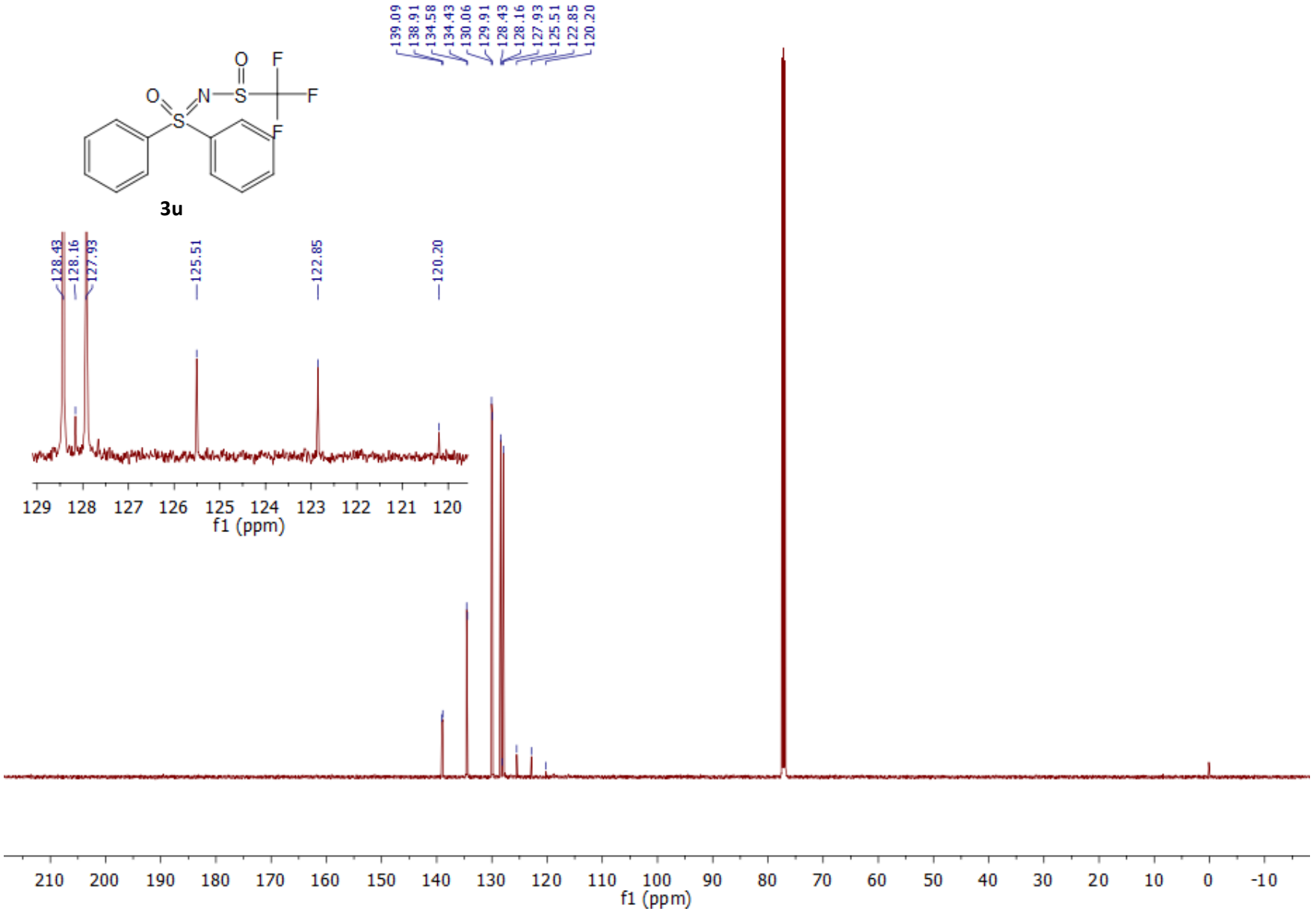

142.18
141.96
135.42
135.34
130.78
130.28
130.16
130.01
128.09
125.44
125.39
122.78
122.73
120.13
120.08
64.98
64.38
4.83
4.69
4.64
4.52
4.20
O
F
O
N
S
S
F
F
Cl
3t
128.09
125.44
125.39
122.78
122.73
120.13
120.08
129 128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

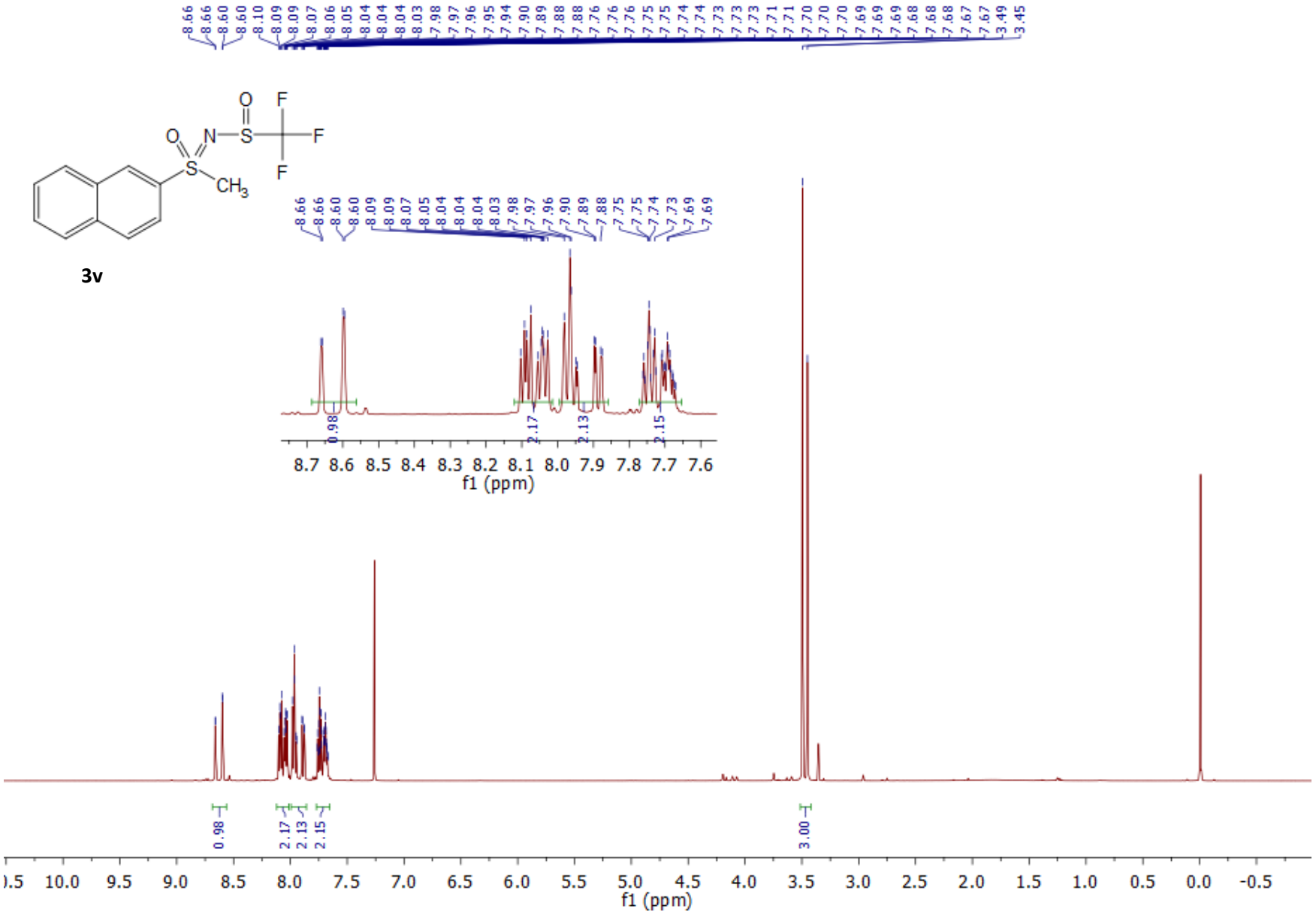

8.04 8.04 8.03 8.03 8.02 8.01 8.01 7.68 7.68 7.68 7.67 7.67 7.66 7.66 7.66 7.65 7.65 7.65 7.64 7.61 7.60 7.59 7.58 7.57 7.57
O F
O N S F
S F
3u
3.96 2.00 4.01
8.0 7.9 7.8 7.7 7.6
f1 (ppm)
3.96 2.00 4.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

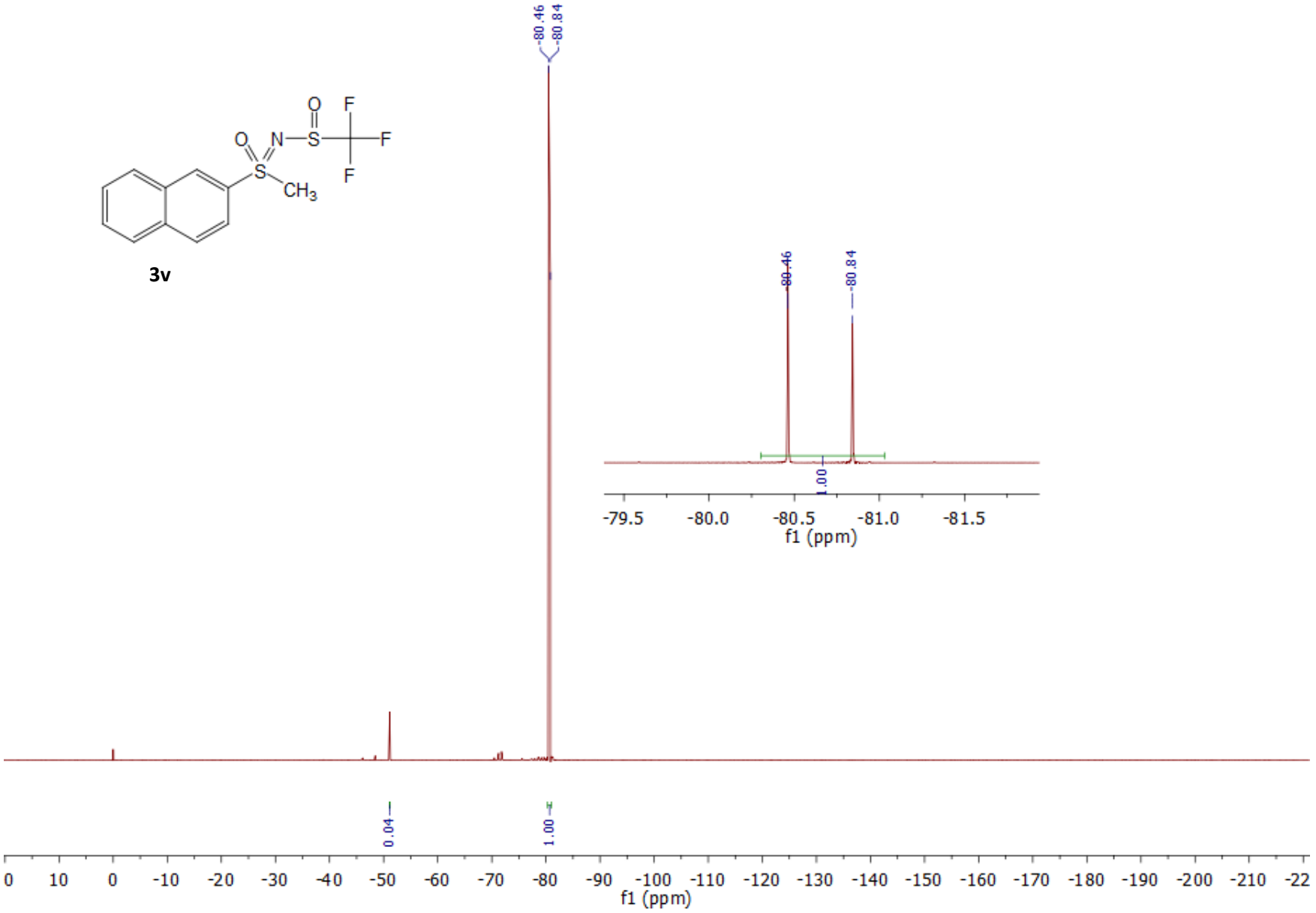
O
F
O
N
S
F
S
F

3u


-80.57
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

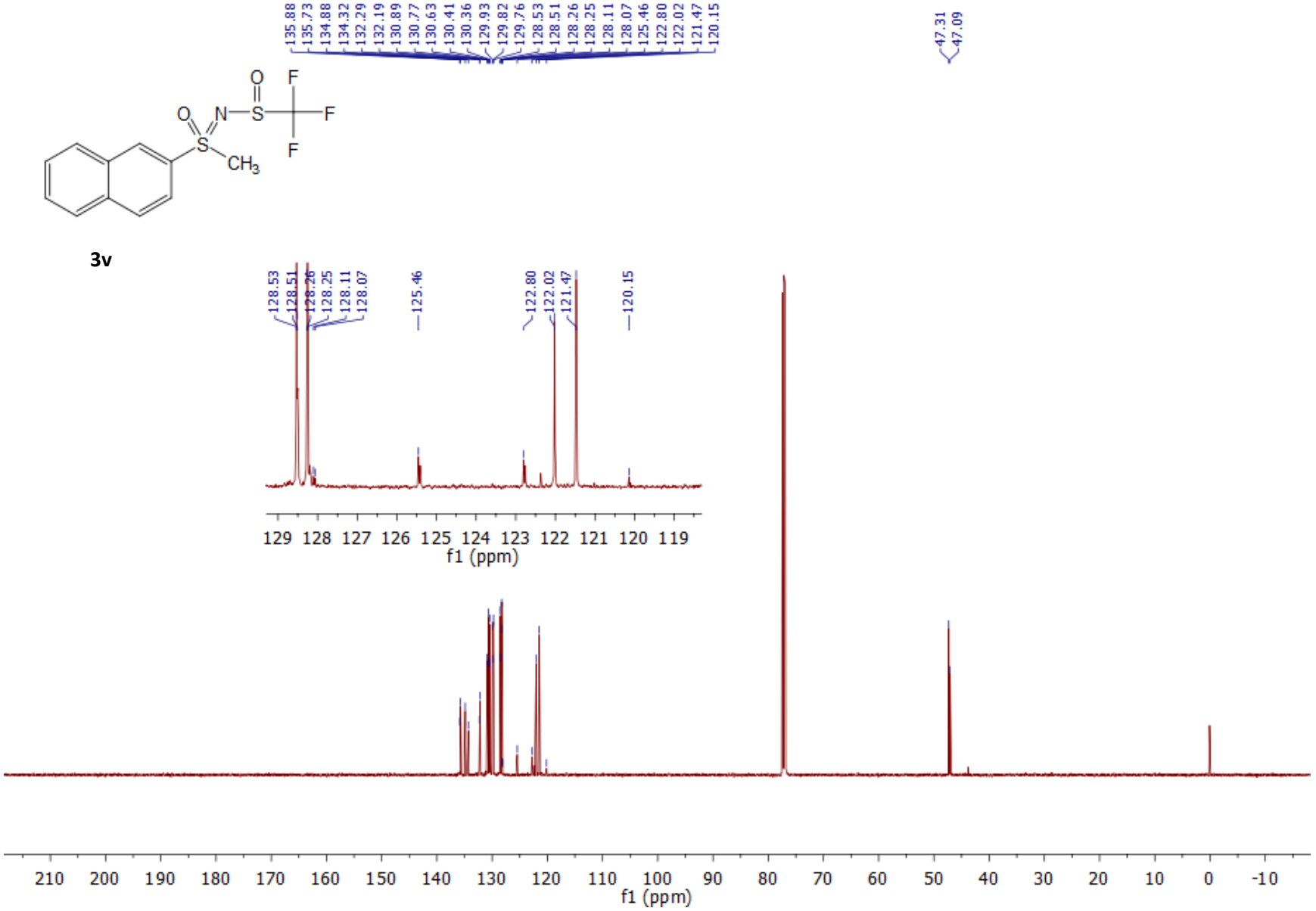

139.09
138.91
134.58
134.43
130.06
129.91
128.43
128.16
127.93
125.51
122.85
120.20
O
F
O
N
S
F
S
F
3u
128.43
128.16
127.93
125.51
122.85
120.20
129 128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

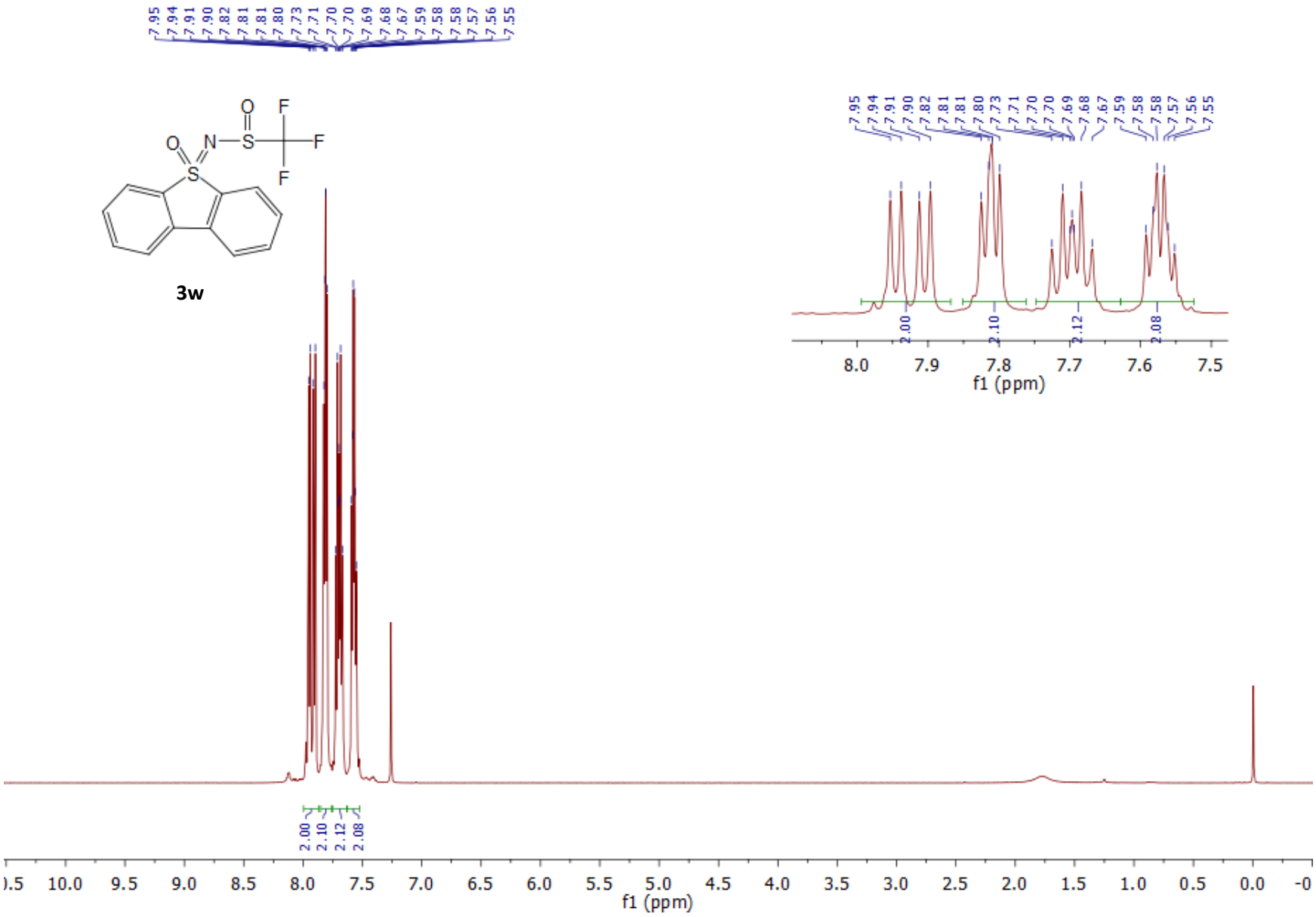

8.66 8.66 8.60 8.60 8.10 8.09 8.09 8.07 8.06 8.05 8.04 8.04 8.04 8.03 7.98 7.97 7.96 7.95 7.94 7.90 7.89 7.88 7.88 7.76 7.76 7.76 7.75 7.75 7.74 7.74 7.73 7.73 7.73 7.71 7.71 7.70 7.70 7.70 7.69 7.69 7.69 7.68 7.68 7.68 7.67 7.67 3.49 3.45
O F O N S F S CH3 F
3v
8.66 8.66 8.60 8.60 8.09 8.09 8.07 8.05 8.04 8.04 8.04 8.03 7.98 7.97 7.96 7.90 7.89 7.88 7.75 7.75 7.74 7.73 7.69 7.69
0.98 2.17 2.13 2.15
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6
f1 (ppm)
0.98 2.17 2.13 2.15 3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


-80.46
-80.84
O
F
O
N
S
F
S
F
CH3
3v
-80.46
-80.84
1.00
-79.5
-80.0
-80.5
-81.0
-81.5
f1 (ppm)
0.04
1.00
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

O
F
O
N
S
F
S
F
CH3

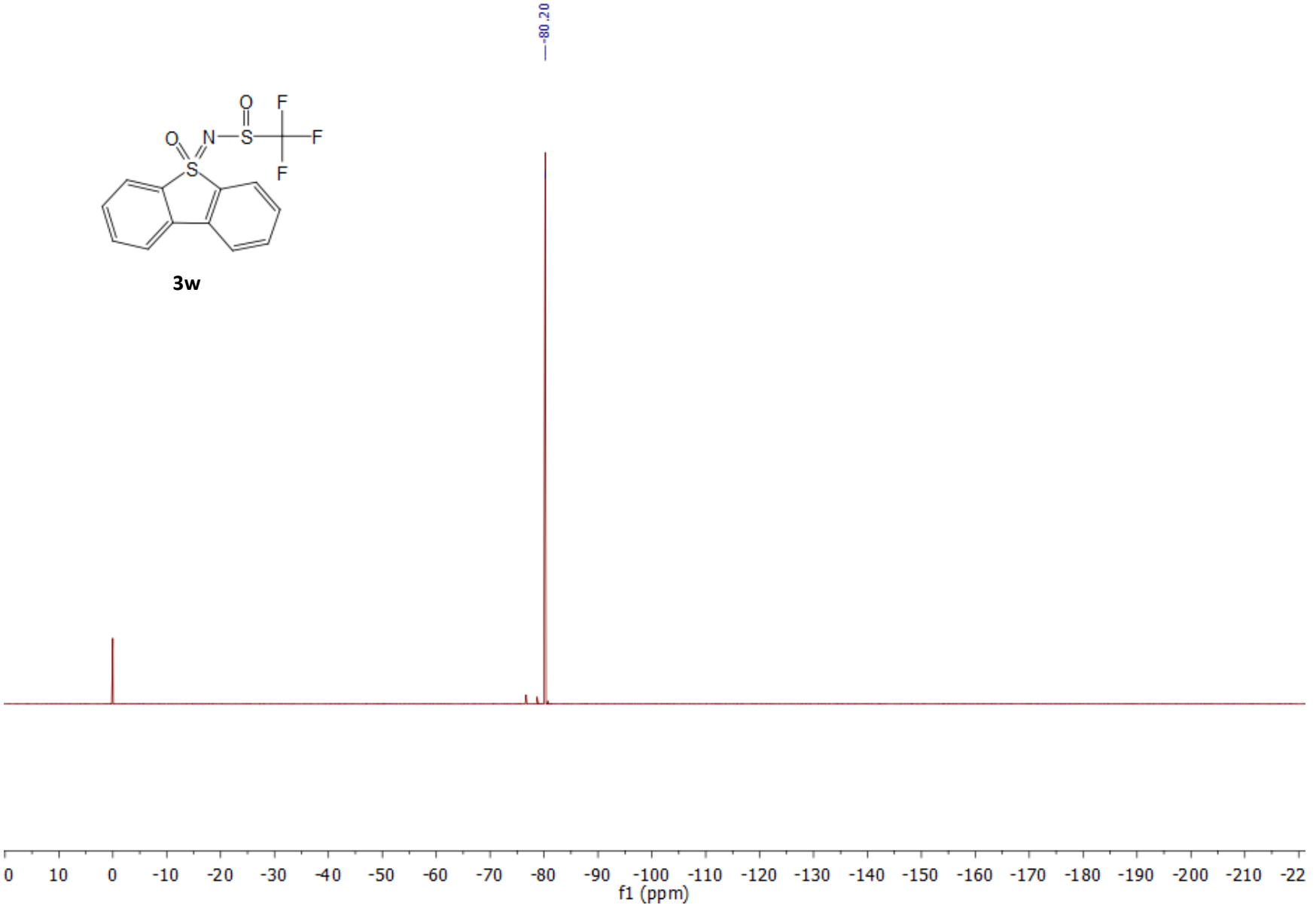
3v

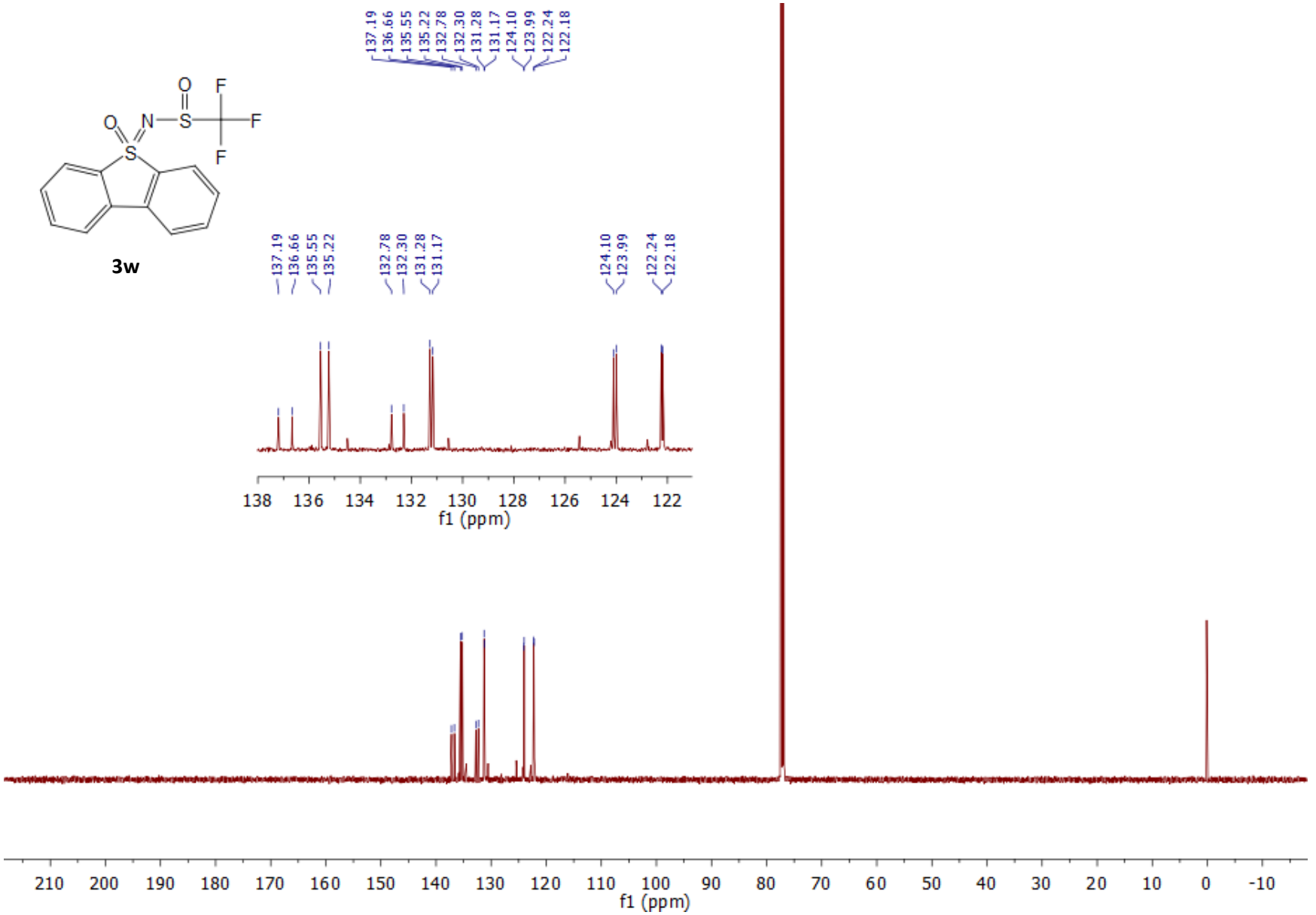

135.88
135.73
134.88
134.32
132.29
132.19
130.89
130.77
130.63
130.41
130.36
129.93
129.82
129.76
128.53
128.51
128.26
128.25
128.11
128.07
125.46
122.80
122.02
121.47
120.15
47.31
47.09
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

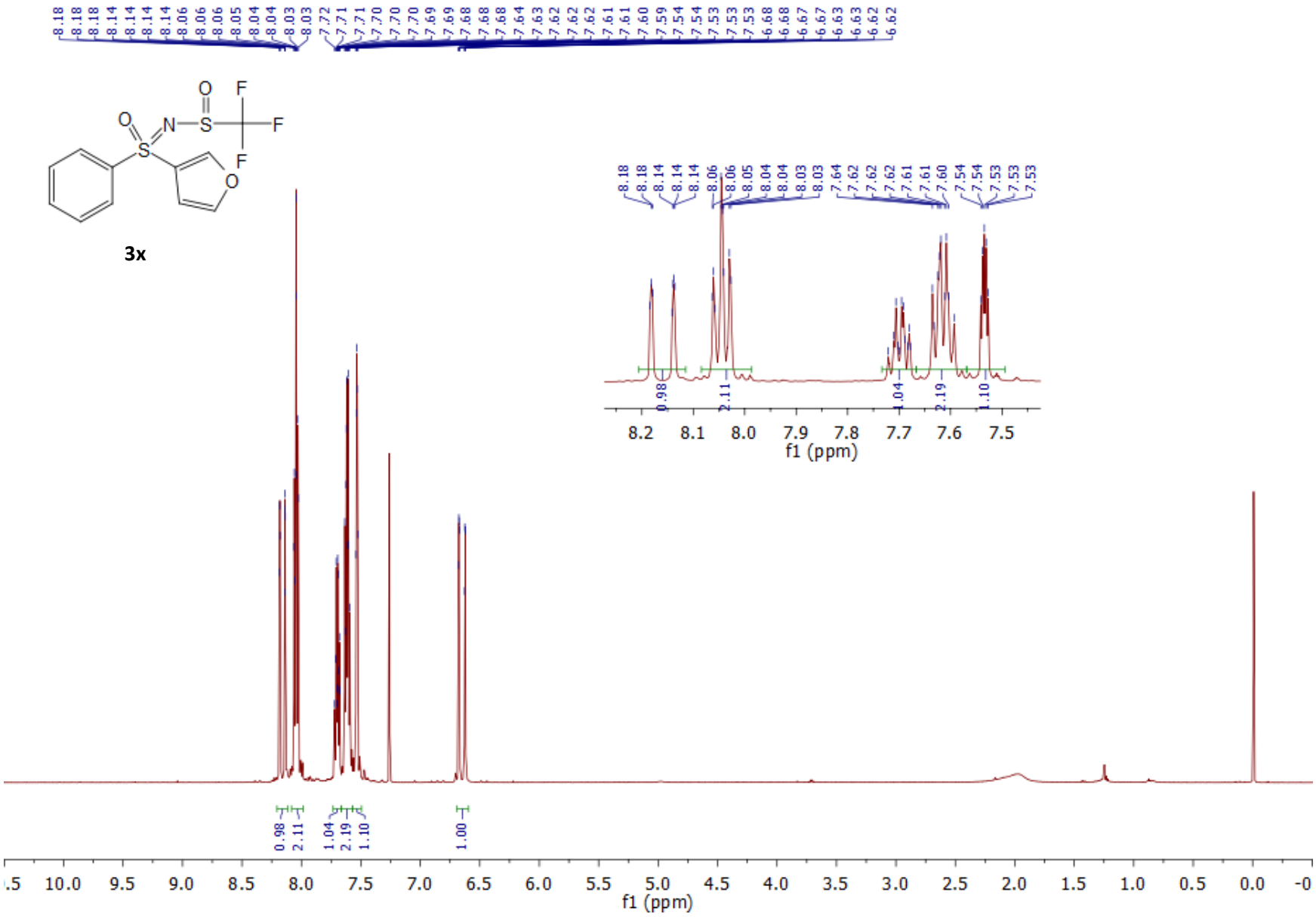

7.95 7.94 7.91 7.90 7.82 7.81 7.81 7.80 7.73 7.71 7.70 7.70 7.69 7.68 7.67 7.59 7.58 7.58 7.57 7.56 7.55
O F
O N S F
S
F
3w
2.00 2.10 2.12 2.08
8.0 7.9 7.8 7.7 7.6 7.5
f1 (ppm)
2.00 2.10 2.12 2.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

O
F
O
N
S
F
S
F

3w

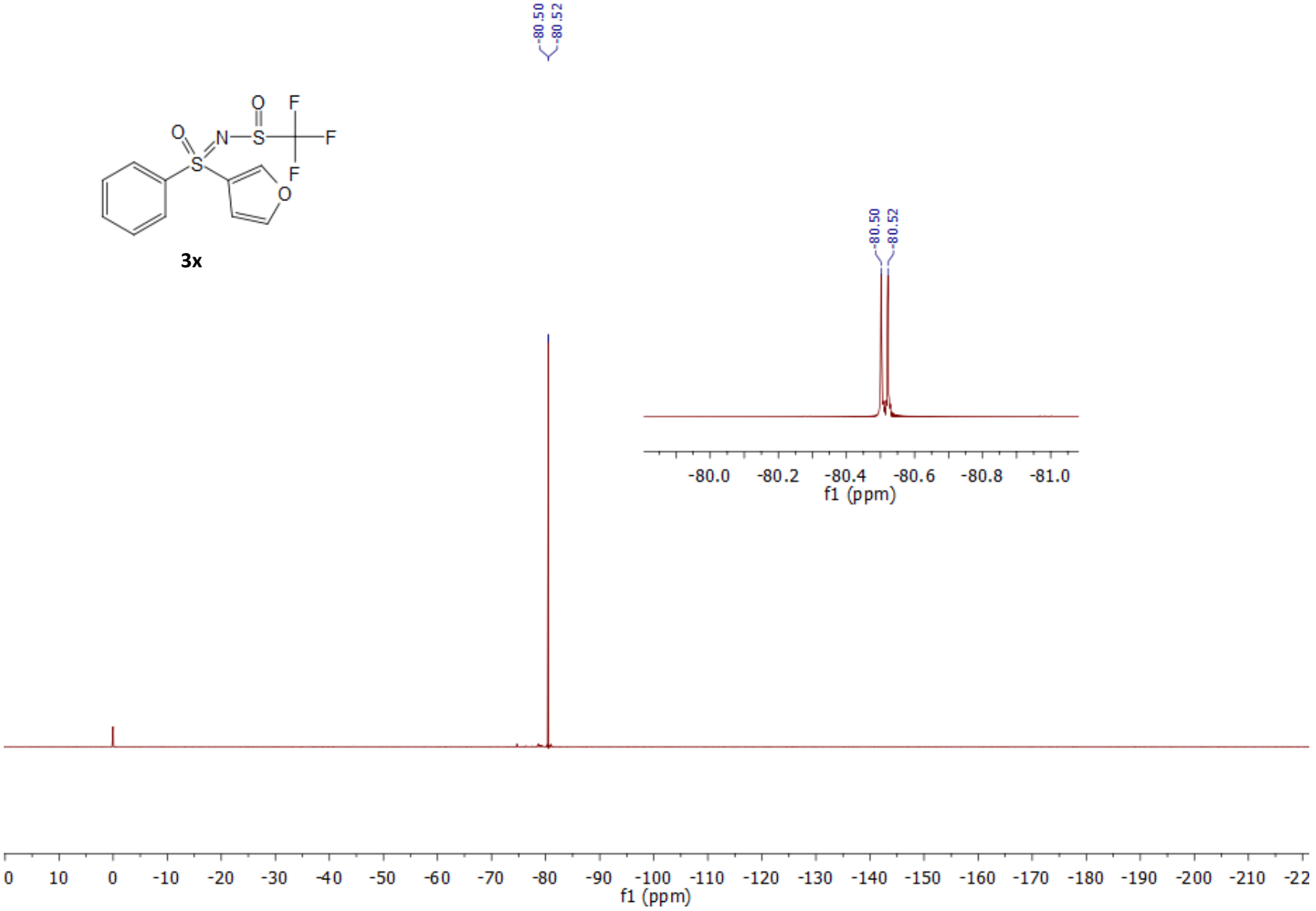

-80.20
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

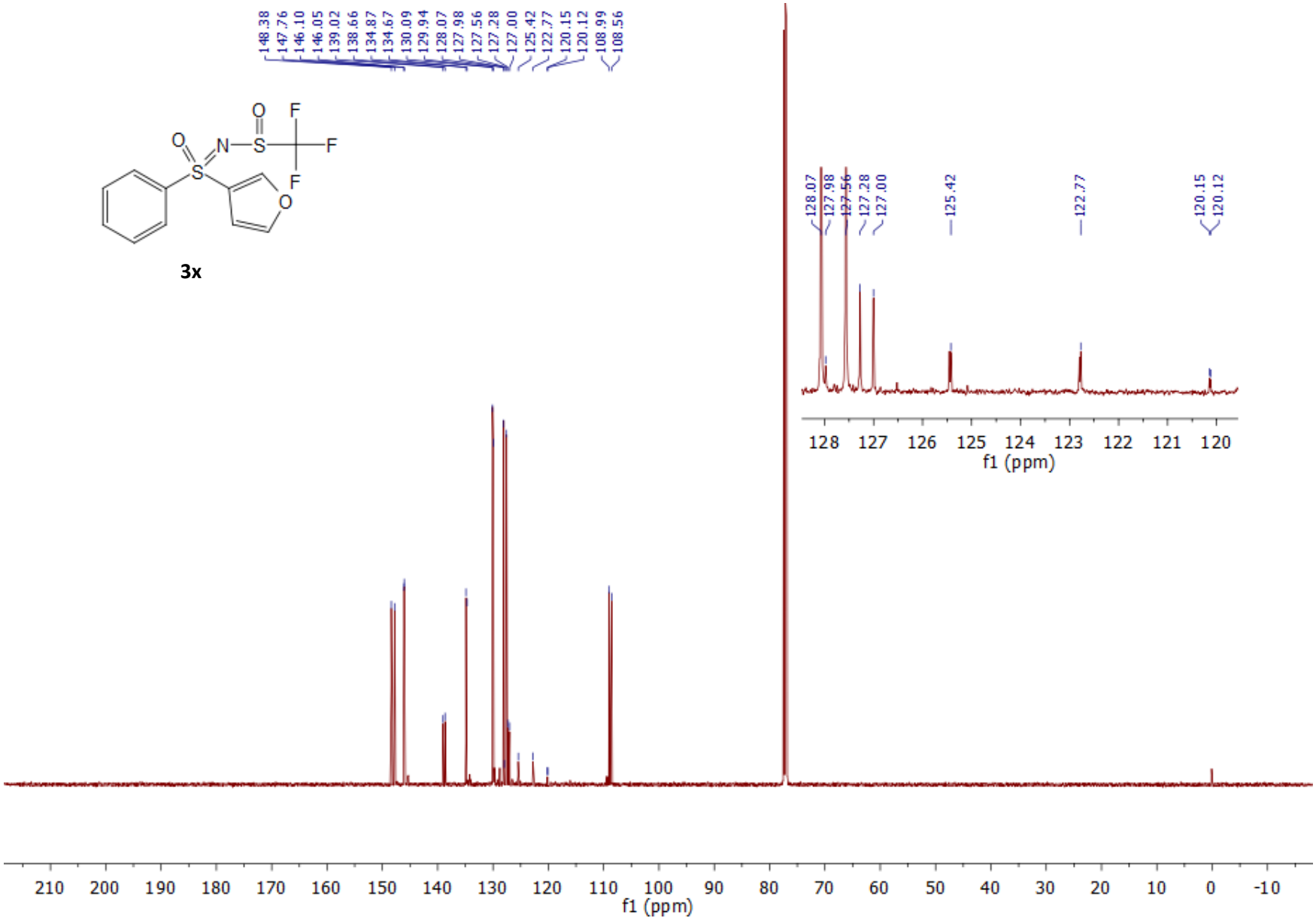

137.19
136.66
135.55
135.22
132.78
132.30
131.28
131.17
124.10
123.99
122.24
122.18
O
F
O
N
S
F
S
F
3w
138
136
134
132
130
128
126
124
122
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

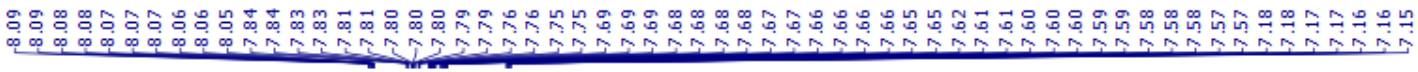

O
F
O
N
S
F
S
F
O
3x
f1 (ppm)
f1 (ppm)

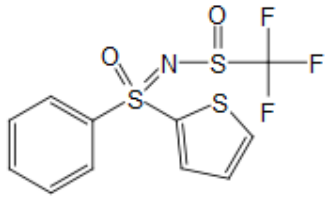
O
F
O
N
S
F
S
F
O

3x

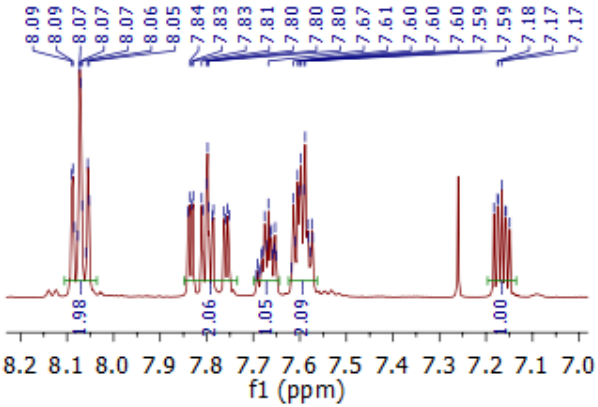

-80.50
-80.52
-80.50
-80.52
-80.0
-80.2
-80.4
-80.6
-80.8
-81.0
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

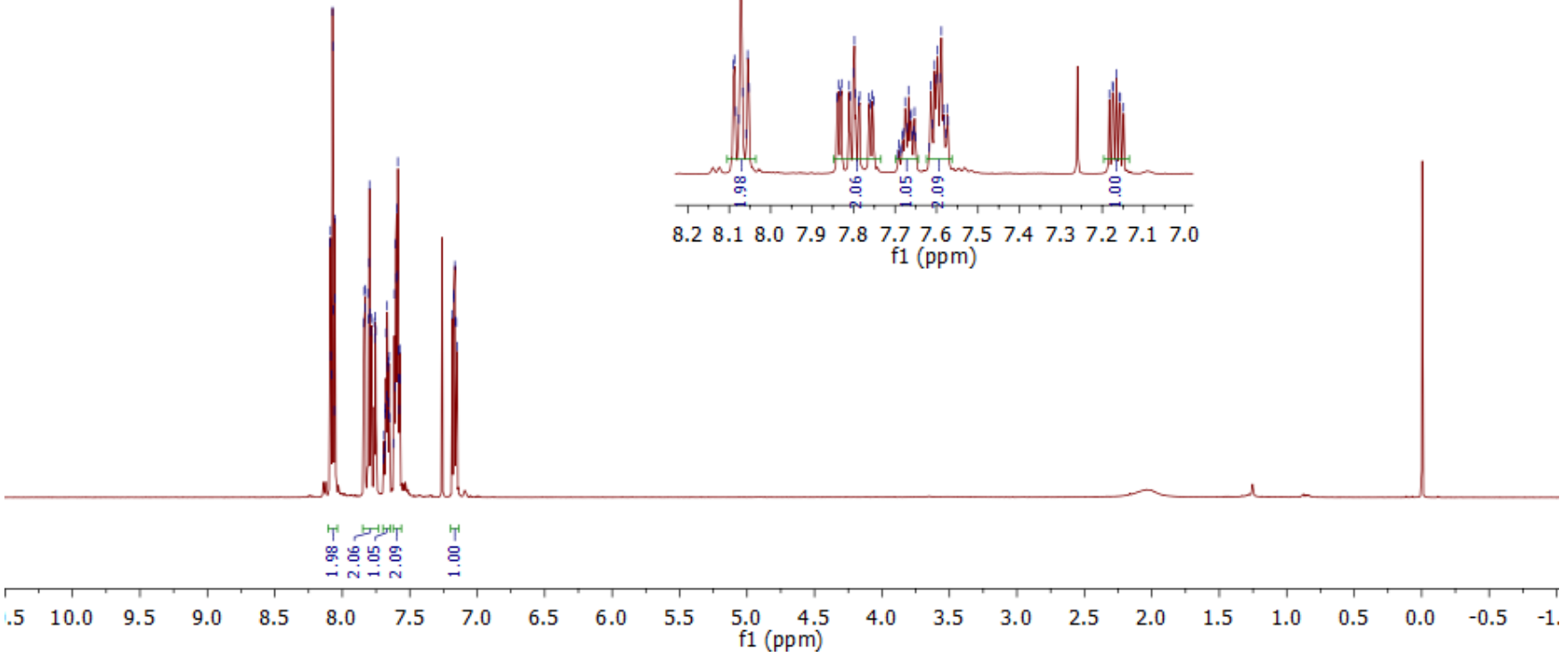

148.38
147.76
146.10
146.05
139.02
138.66
134.87
134.67
130.09
129.94
128.07
127.98
127.56
127.28
127.00
125.42
122.77
120.15
120.12
108.99
108.56
O
F
O
N
S
S
F
F
O
3x
128.07
127.98
127.56
127.28
127.00
125.42
122.77
120.15
120.12
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)





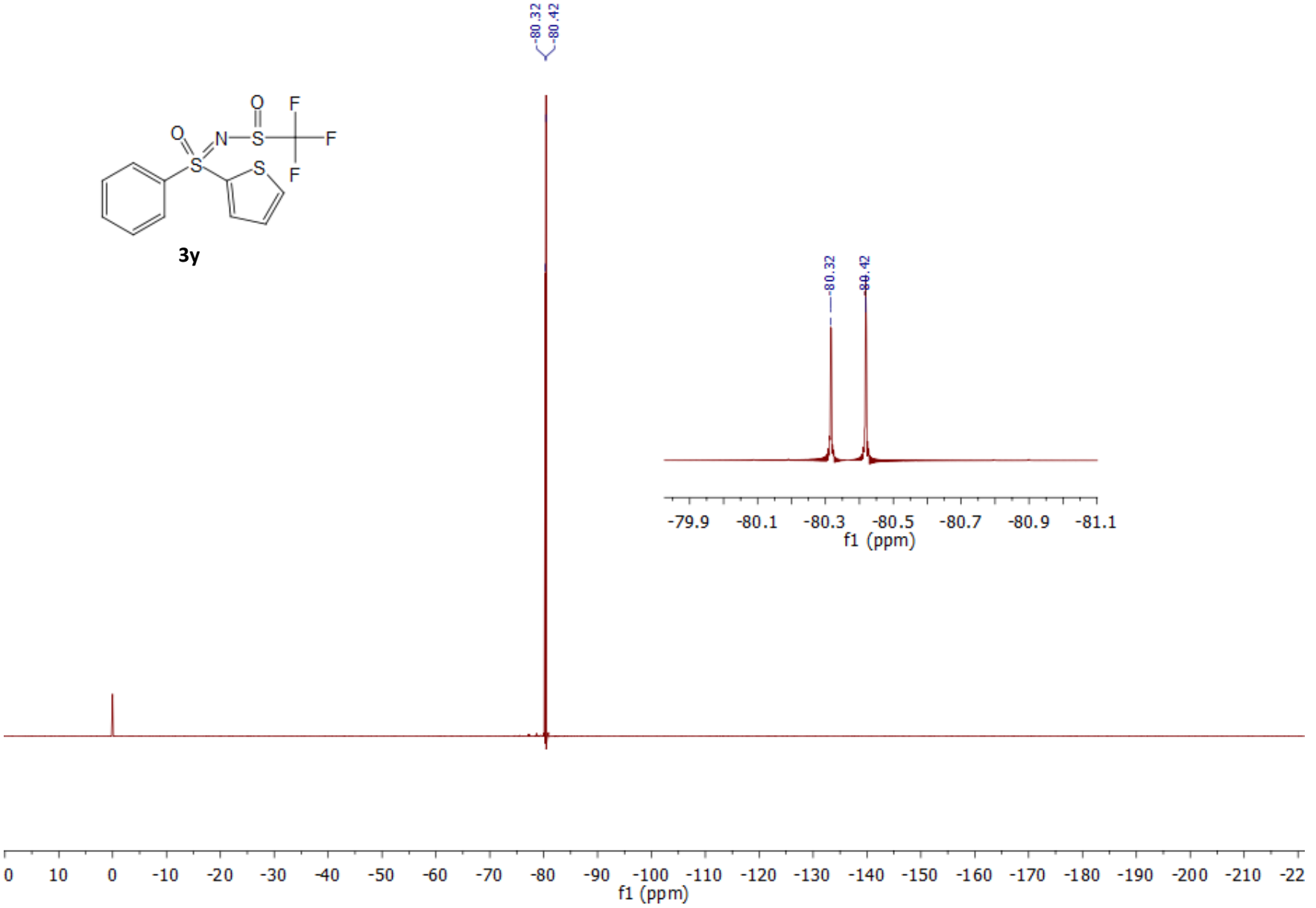
3y

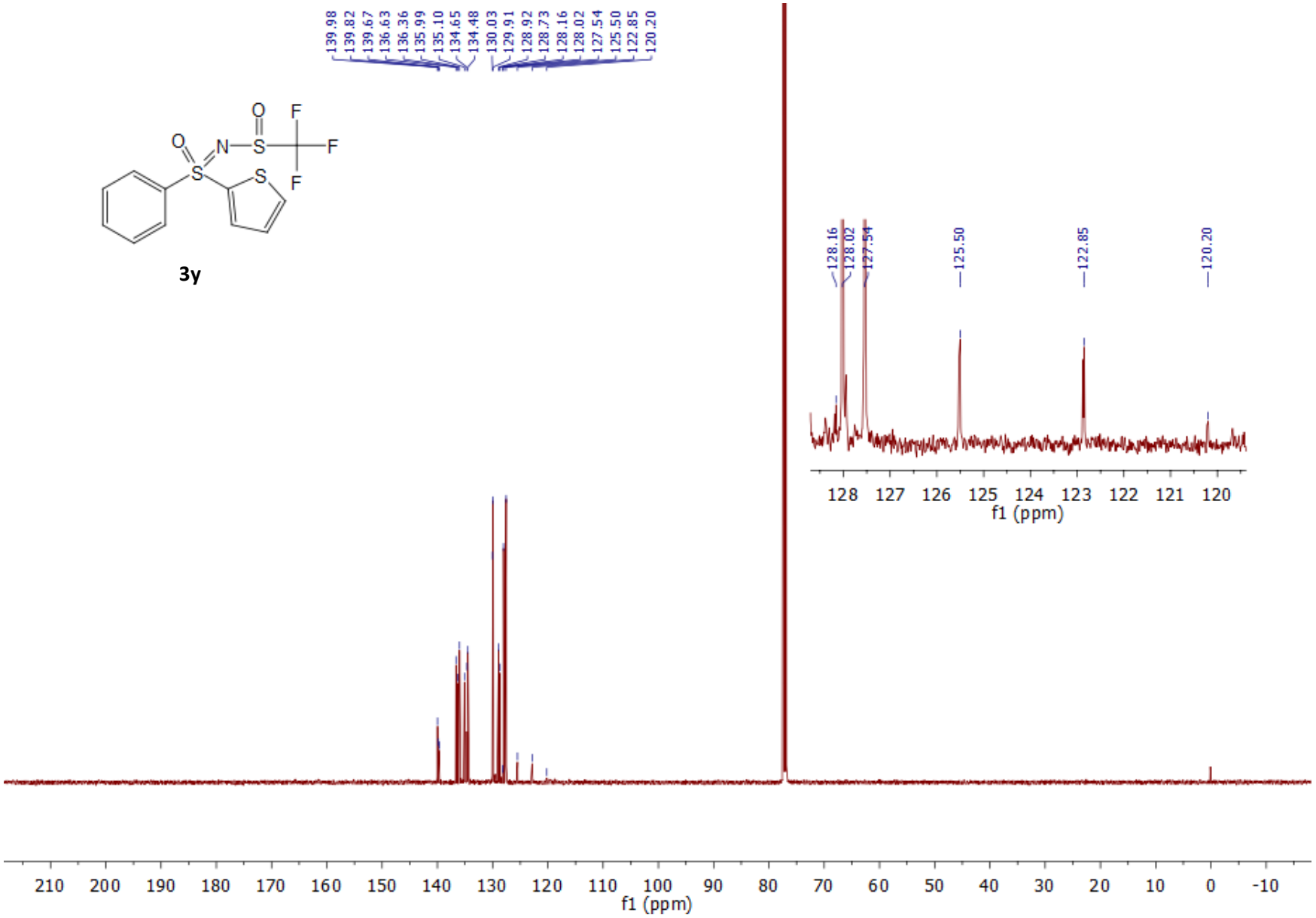

1.98
2.06
1.05
2.09
1.00
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)

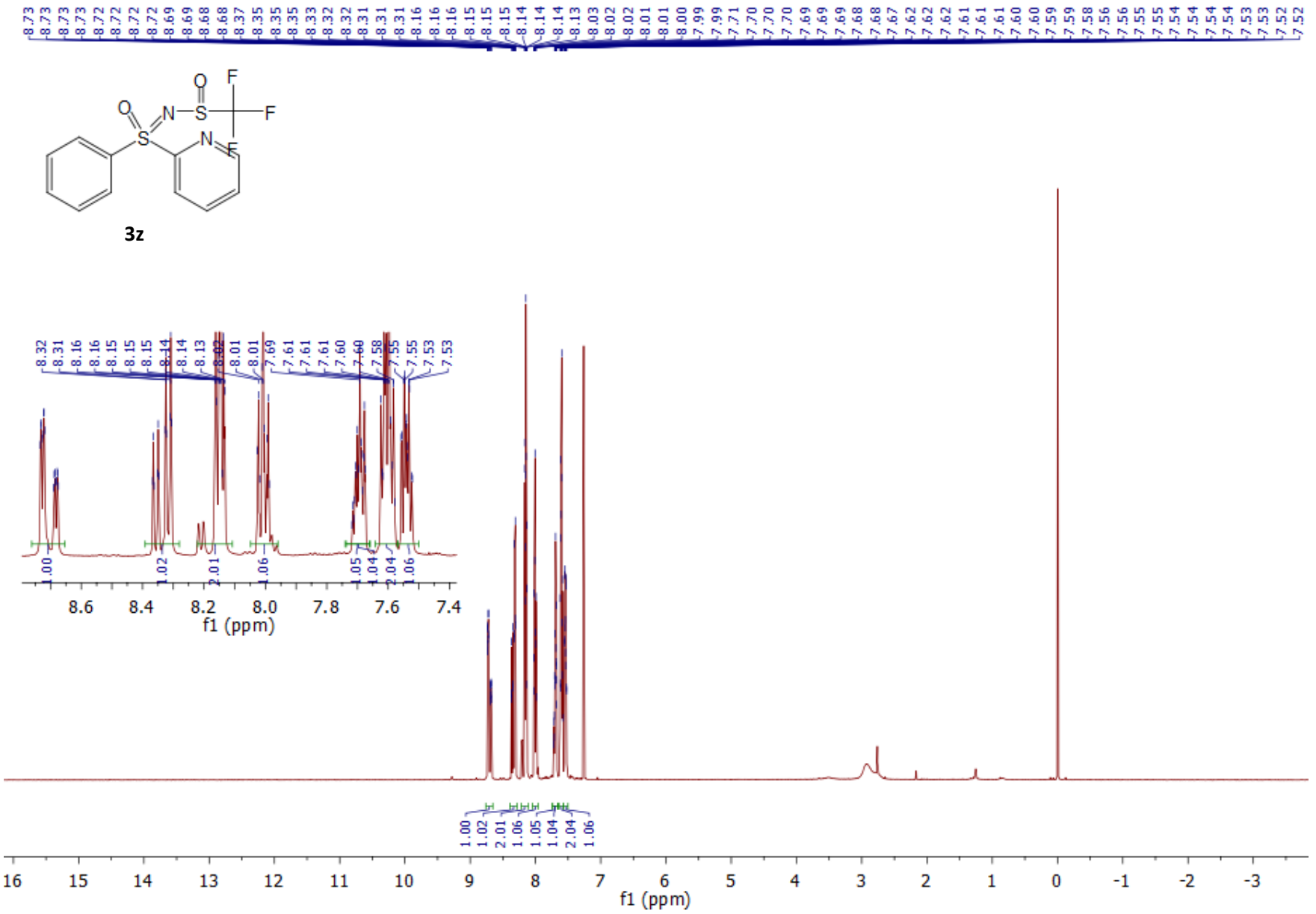

1.98
2.06
1.05
2.09
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

O
F
O
N
S
F
S
S
F

3y

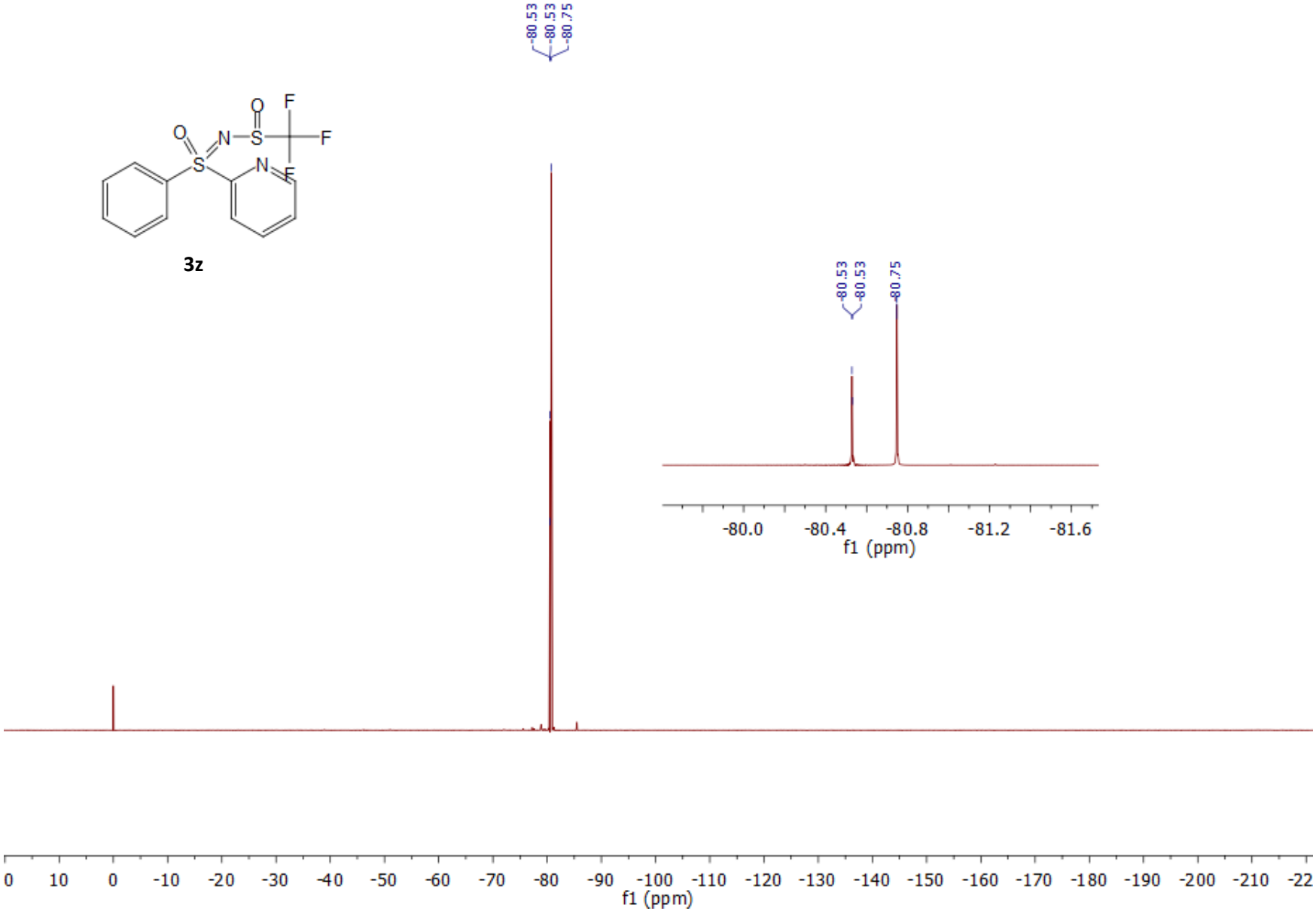

-80.32
-80.42
-80.32
-80.42
-79.9
-80.1
-80.3
-80.5
-80.7
-80.9
-81.1
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

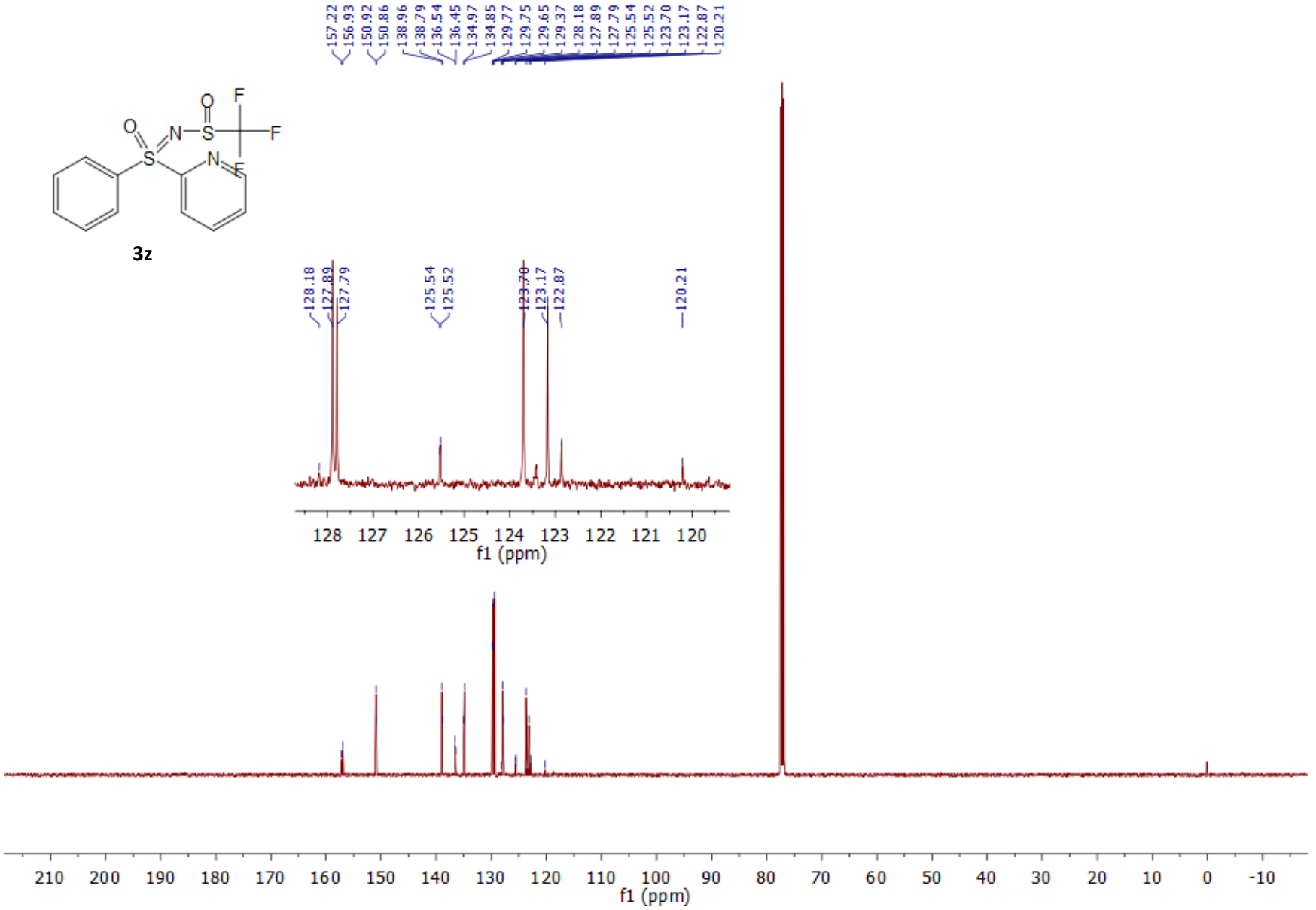

139.98
139.82
139.67
136.63
136.36
135.99
135.10
134.65
134.48
130.03
129.91
128.92
128.73
128.16
128.02
127.54
125.50
122.85
120.20
O
F
O
N
S
F
S
S
F
3y
128.16
128.02
127.54
125.50
122.85
120.20
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

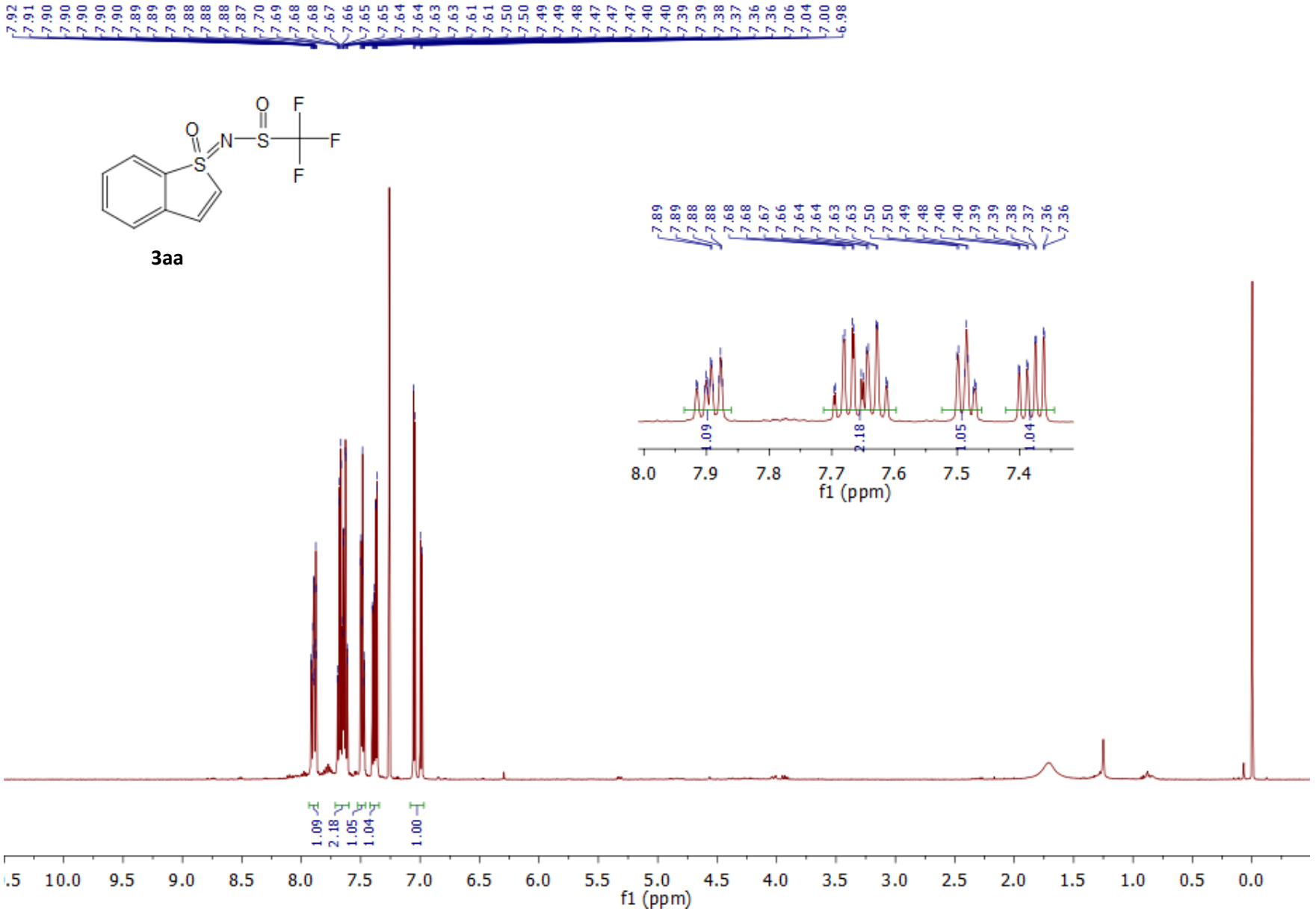

O
F
O
N
S
F
S
N
F
3z
f1 (ppm)
f1 (ppm)

O
F
O
N
S
F
S
N
F

3z

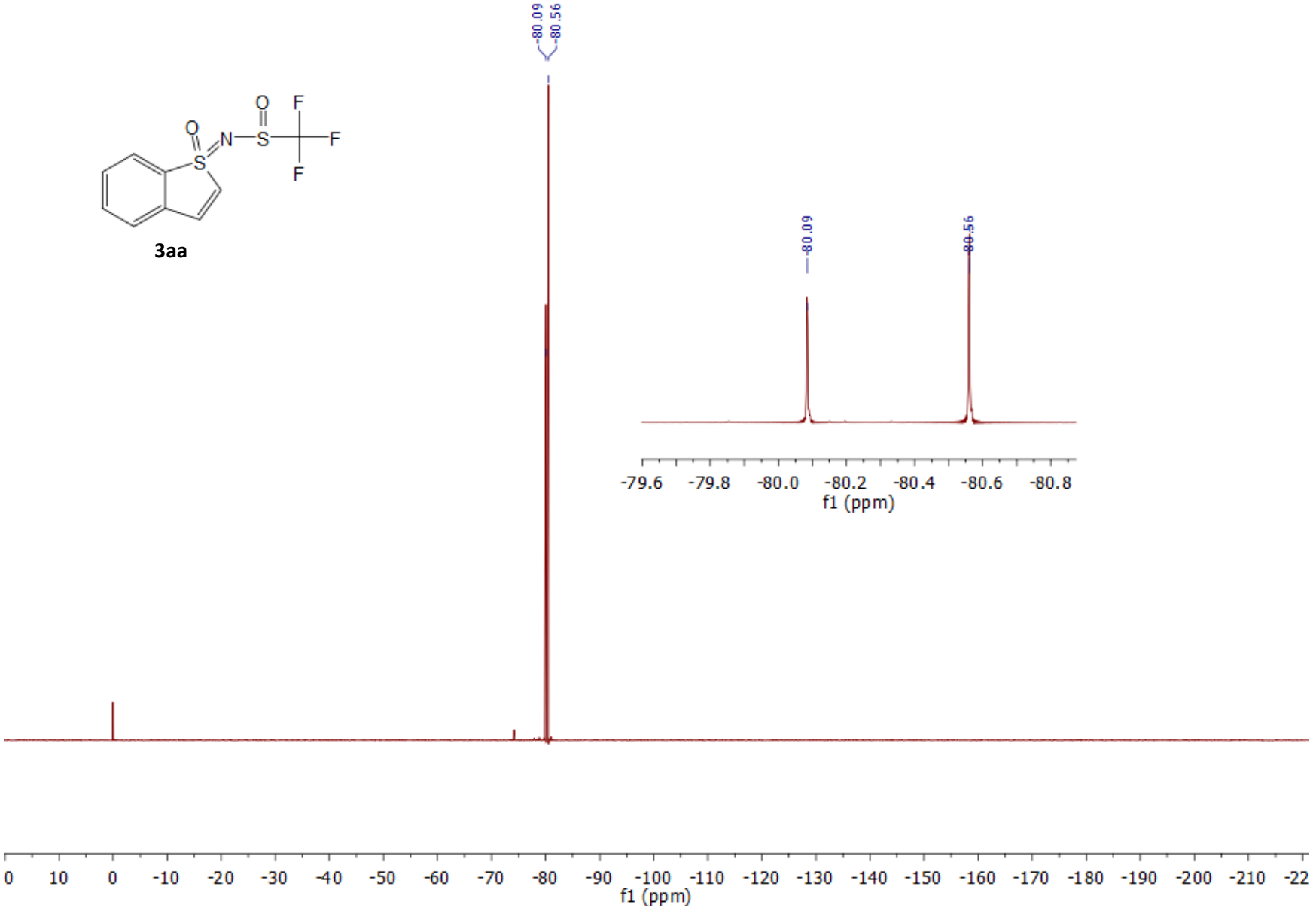

-80.53
-80.53
-80.75
-80.53
-80.53
-80.75
-80.0
-80.4
-80.8
-81.2
-81.6
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

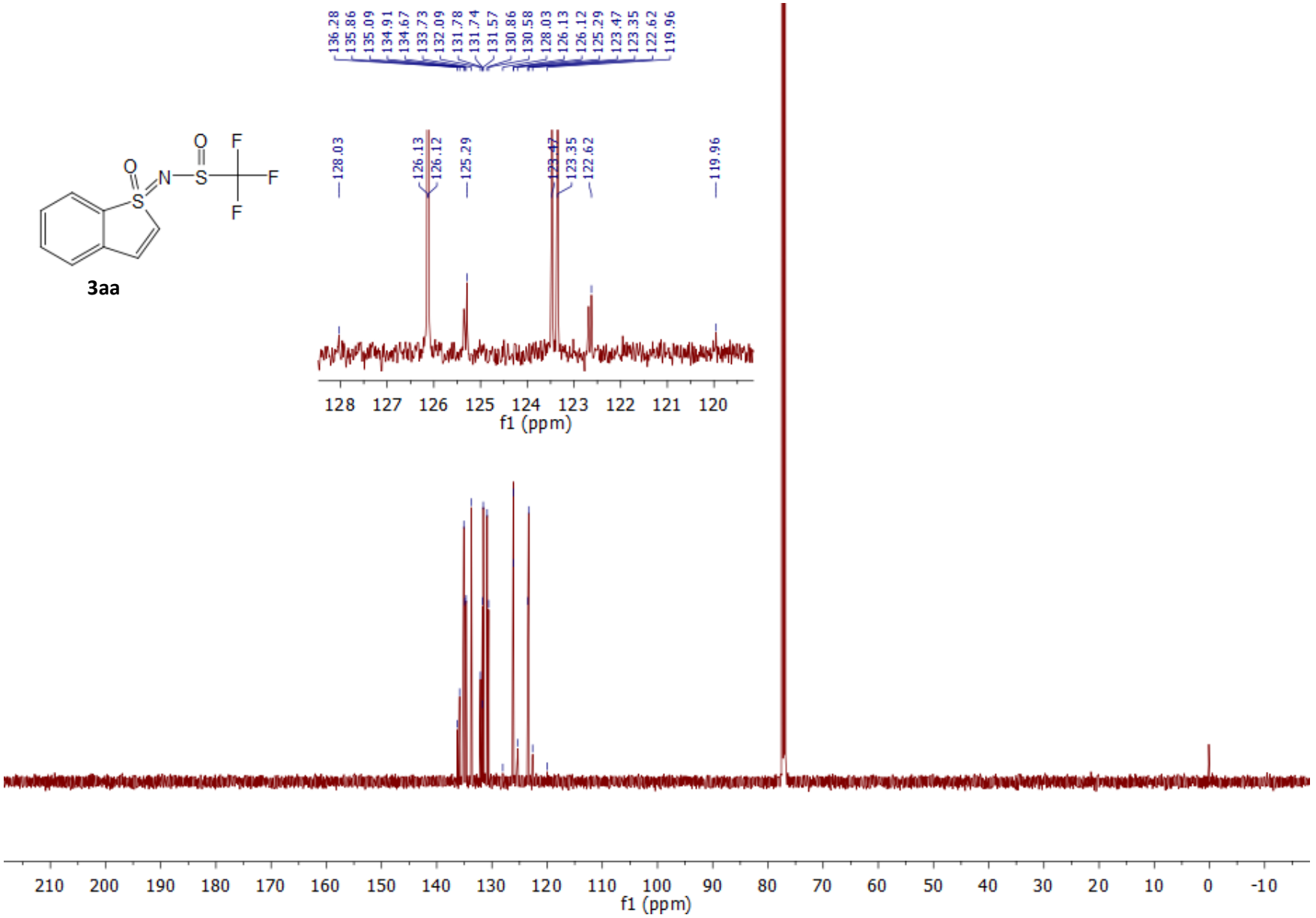

157.22
156.93
150.92
150.86
138.96
138.79
136.54
136.45
134.97
134.85
129.77
129.75
129.65
129.37
128.18
127.89
127.79
125.54
125.52
123.70
123.17
122.87
120.21
O
O
F
N
S
F
S
N
F
3z
128.18
127.89
127.79
125.54
125.52
123.70
123.17
122.87
120.21
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.92 7.91 7.90 7.90 7.90 7.90 7.90 7.89 7.89 7.89 7.88 7.88 7.88 7.87 7.70 7.69 7.68 7.68 7.67 7.66 7.65 7.65 7.64 7.64 7.63 7.63 7.61 7.61 7.50 7.50 7.49 7.49 7.48 7.47 7.47 7.47 7.40 7.40 7.39 7.39 7.38 7.37 7.36 7.36 7.06 7.04 7.00 6.98
O F O N S F F S
3aa
7.89 7.89 7.88 7.88 7.68 7.68 7.67 7.66 7.64 7.64 7.63 7.63 7.50 7.50 7.49 7.48 7.40 7.40 7.39 7.39 7.38 7.37 7.36 7.36
1.09 2.18 1.05 1.04
8.0 7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)
1.09 2.18 1.05 1.04 1.00
.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

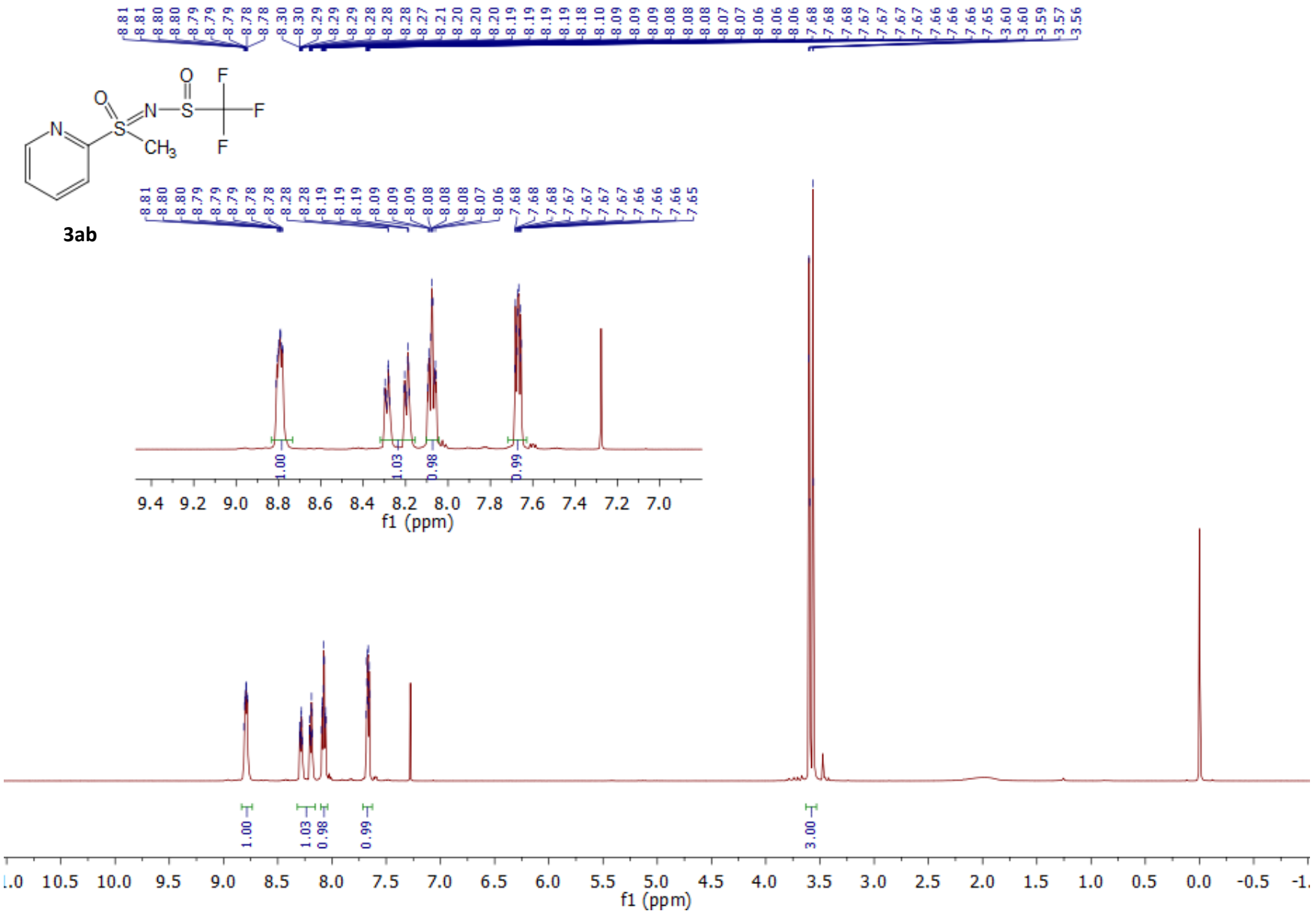
O
F
O
N
S
F
S
F

3aa


-80.09
-80.56
-80.09
-80.56
-79.6
-79.8
-80.0
-80.2
-80.4
-80.6
-80.8
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

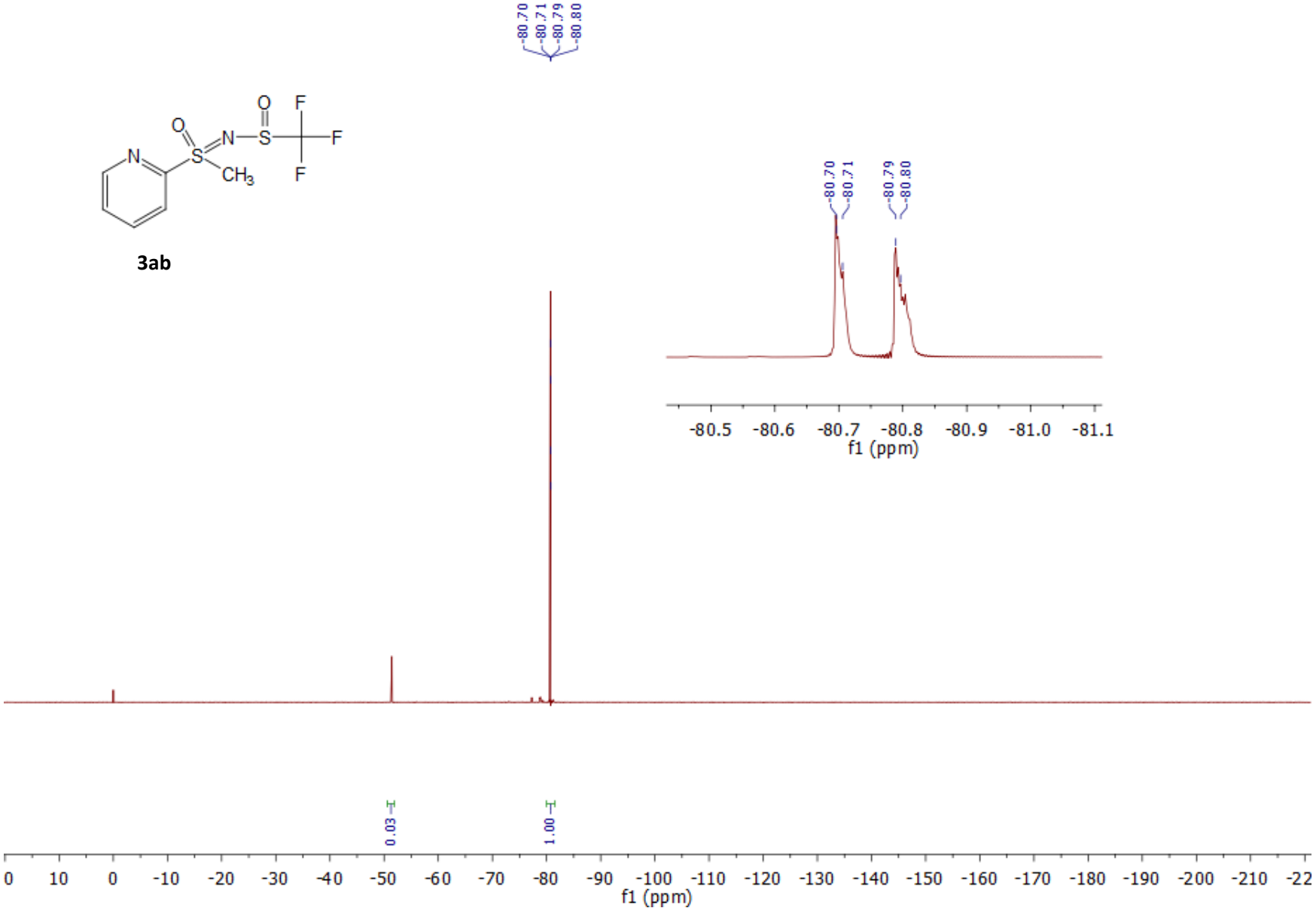

136.28
135.86
135.09
134.91
134.67
133.73
132.09
131.78
131.74
131.57
130.86
130.58
128.03
126.13
126.12
125.29
123.47
123.35
122.62
119.96
O
F
O
N
S
F
S
F
128.03
126.13
126.12
125.29
123.47
123.35
122.62
119.96
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

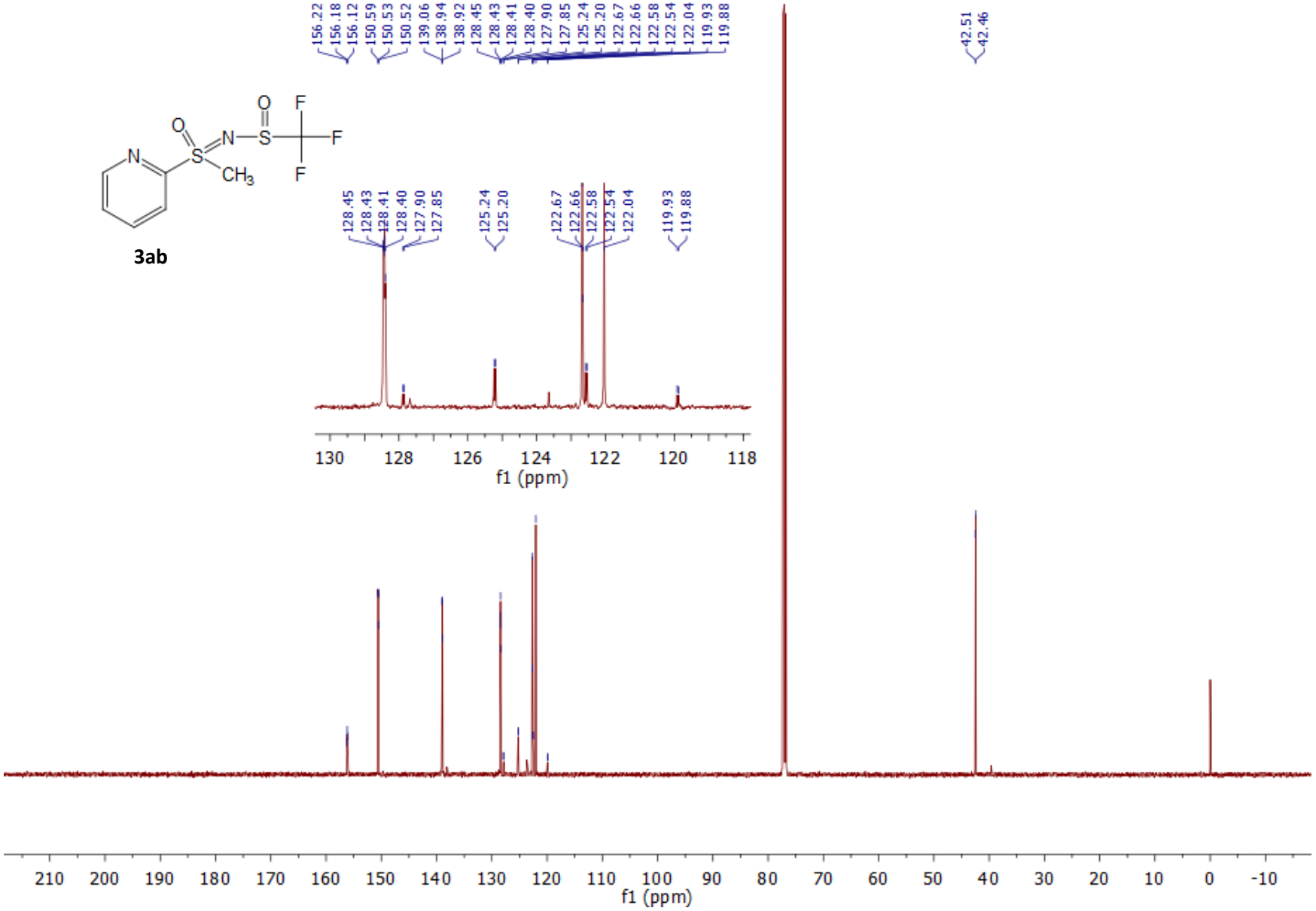
3aa

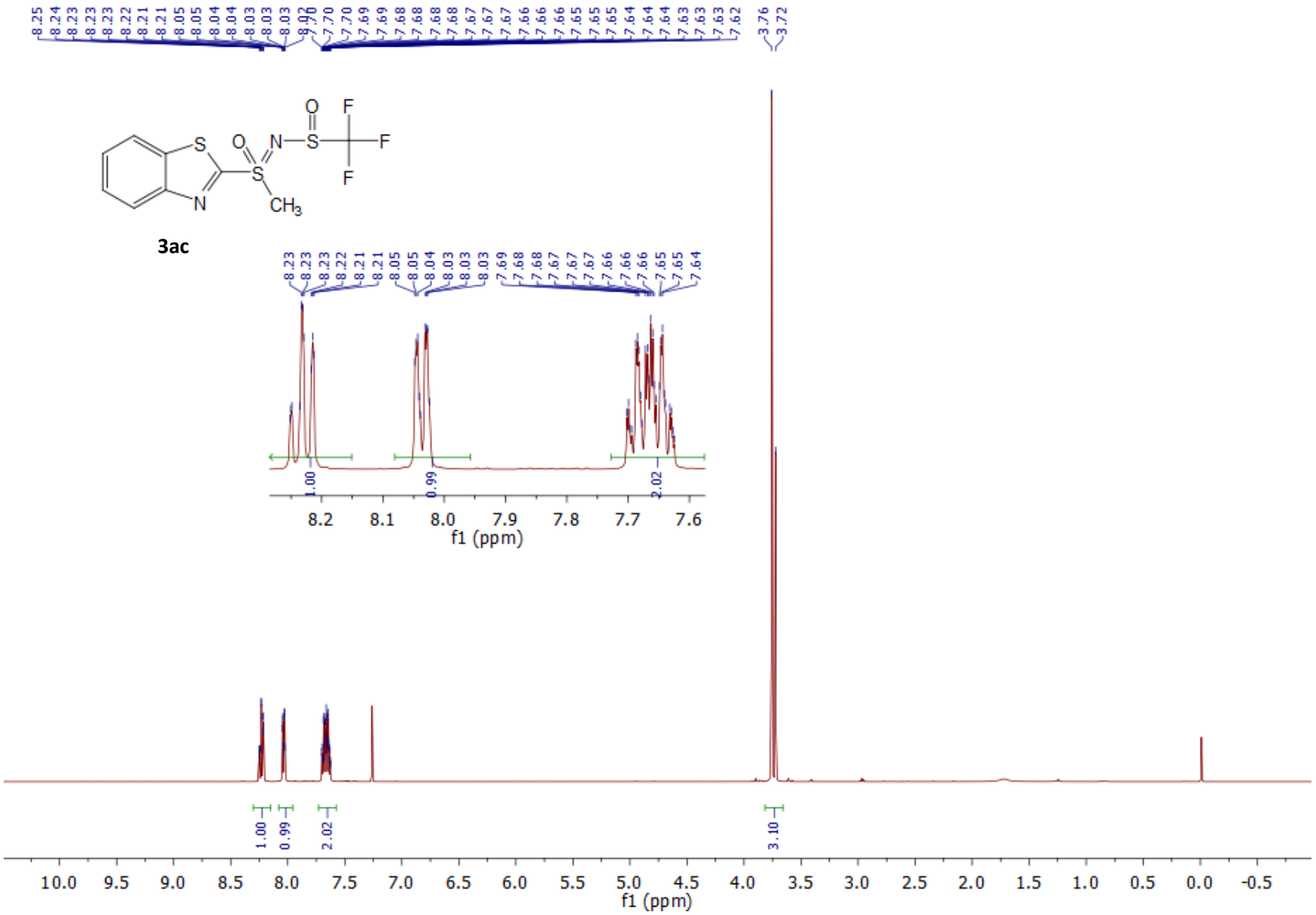

3ab
f1 (ppm)
f1 (ppm)

O
F
O
N
S
F
N
S
F
CH3

3ab

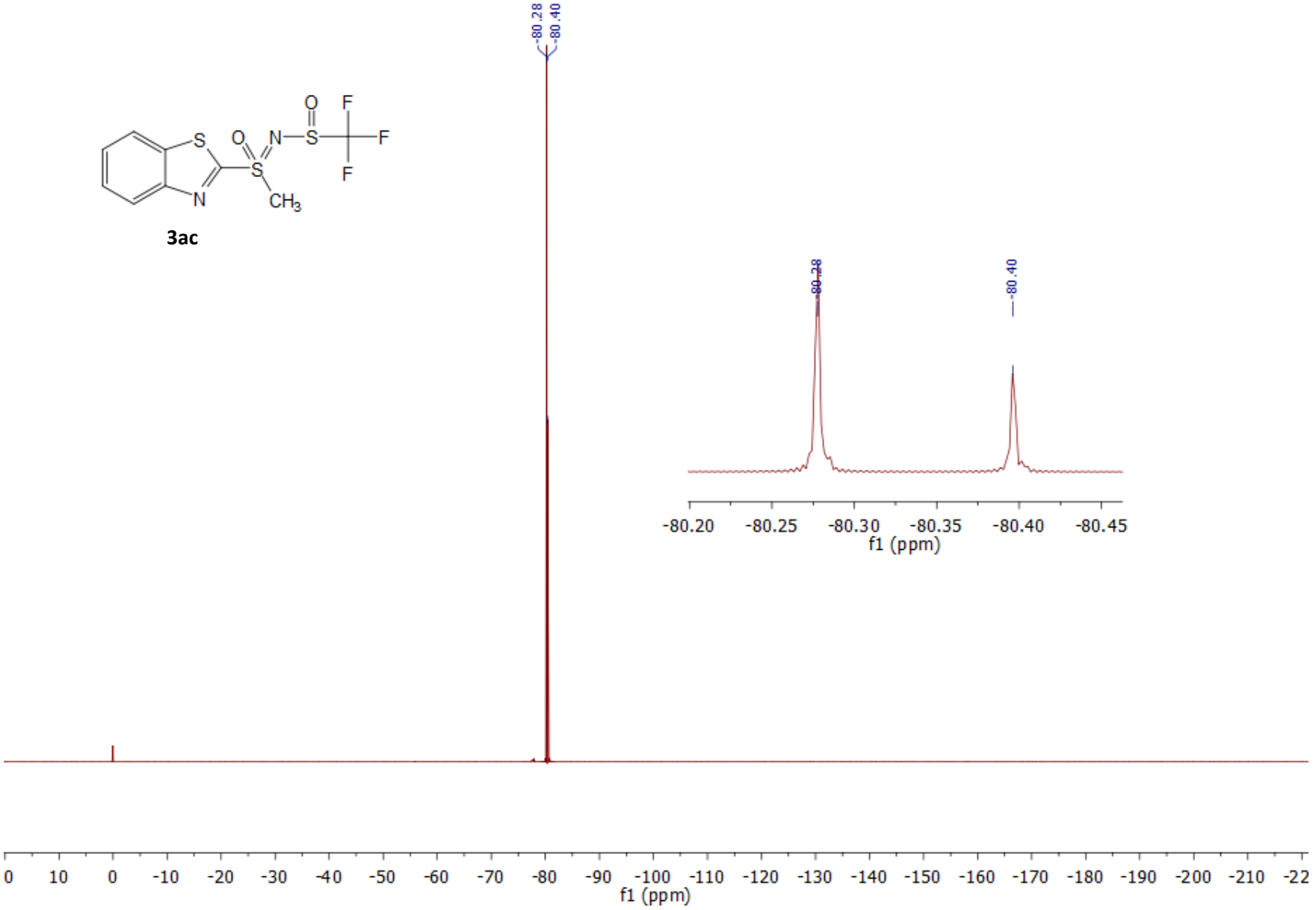

-80.70
-80.71
-80.79
-80.80
-80.70
-80.71
-80.79
-80.80
-80.5
-80.6
-80.7
-80.8
-80.9
-81.0
-81.1
f1 (ppm)
0.03
1.00
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

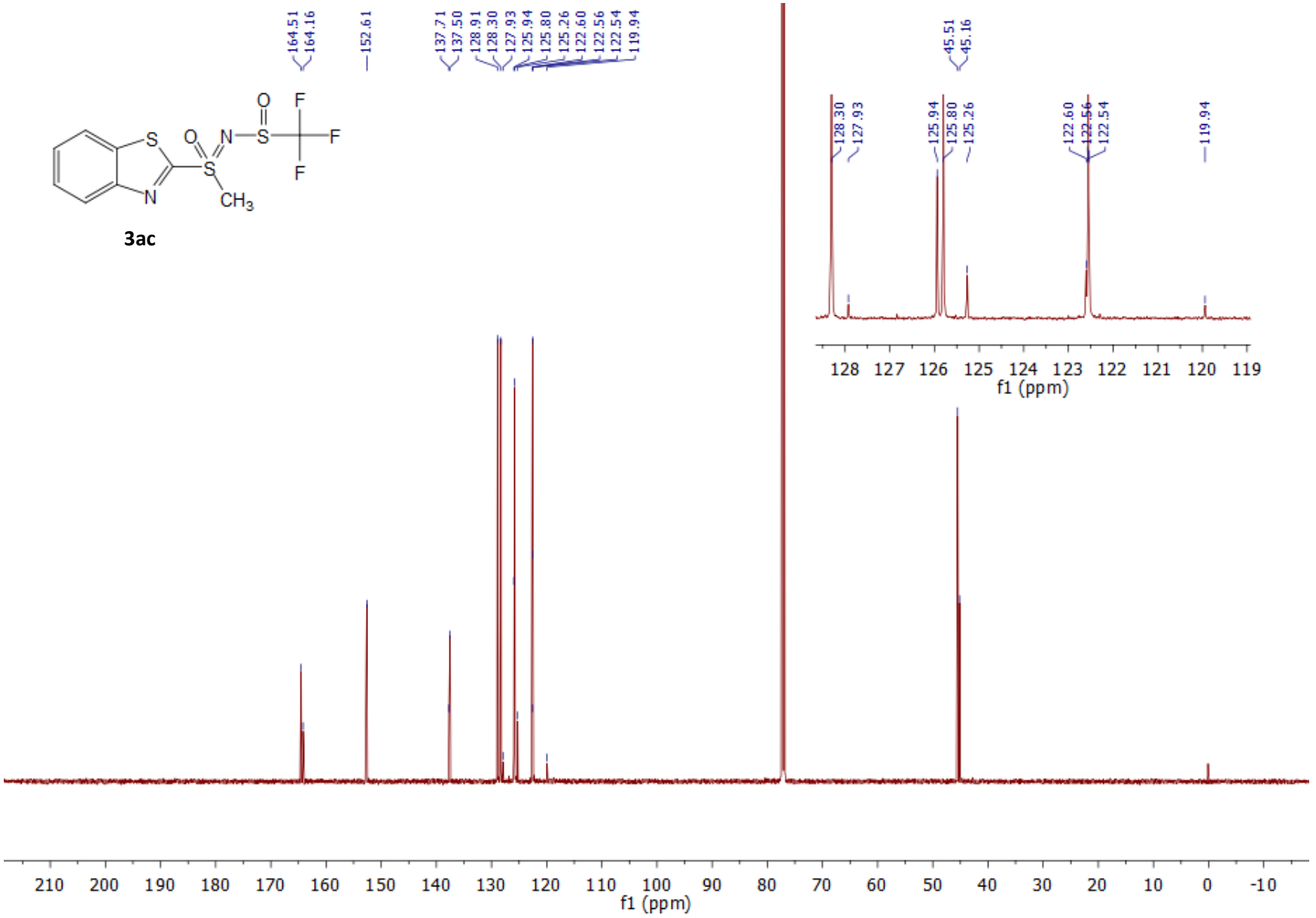

156.22
156.18
156.12
150.59
150.53
150.52
139.06
138.94
138.92
128.45
128.43
128.41
128.40
127.90
127.85
125.24
125.20
122.67
122.66
122.58
122.54
122.04
119.93
119.88
42.51
42.46
O
F
O
N
S
F
N
S
F
CH3
3ab
128.45
128.43
128.41
128.40
127.90
127.85
125.24
125.20
122.67
122.66
122.58
122.54
122.04
119.93
119.88
130
128
126
124
122
120
118
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

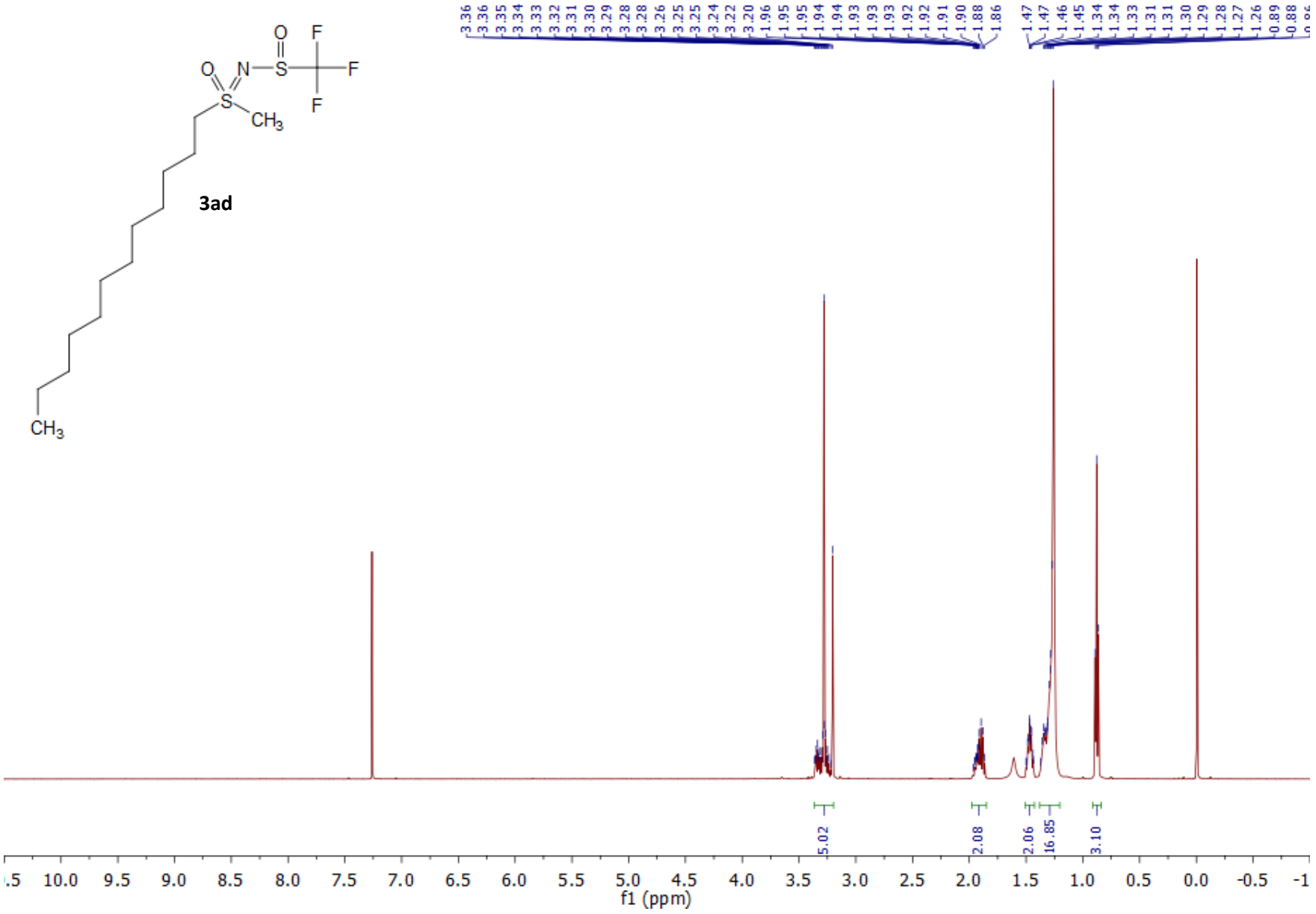

8.25 8.24 8.23 8.23 8.23 8.22 8.21 8.21 8.05 8.05 8.04 8.04 8.03 8.03 8.03 8.02 7.70 7.70 7.69 7.69 7.68 7.68 7.68 7.67 7.67 7.67 7.66 7.66 7.65 7.65 7.64 7.64 7.63 7.63 7.62 3.76 3.72
O F
S O N S F
S F
N CH3
3ac
8.23 8.23 8.23 8.22 8.21 8.21 8.05 8.05 8.04 8.03 8.03 8.03 7.69 7.68 7.67 7.67 7.67 7.66 7.66 7.65 7.65 7.64
1.00 0.99 2.02
8.2 8.1 8.0 7.9 7.8 7.7 7.6
f1 (ppm)
1.00 0.99 2.02 3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

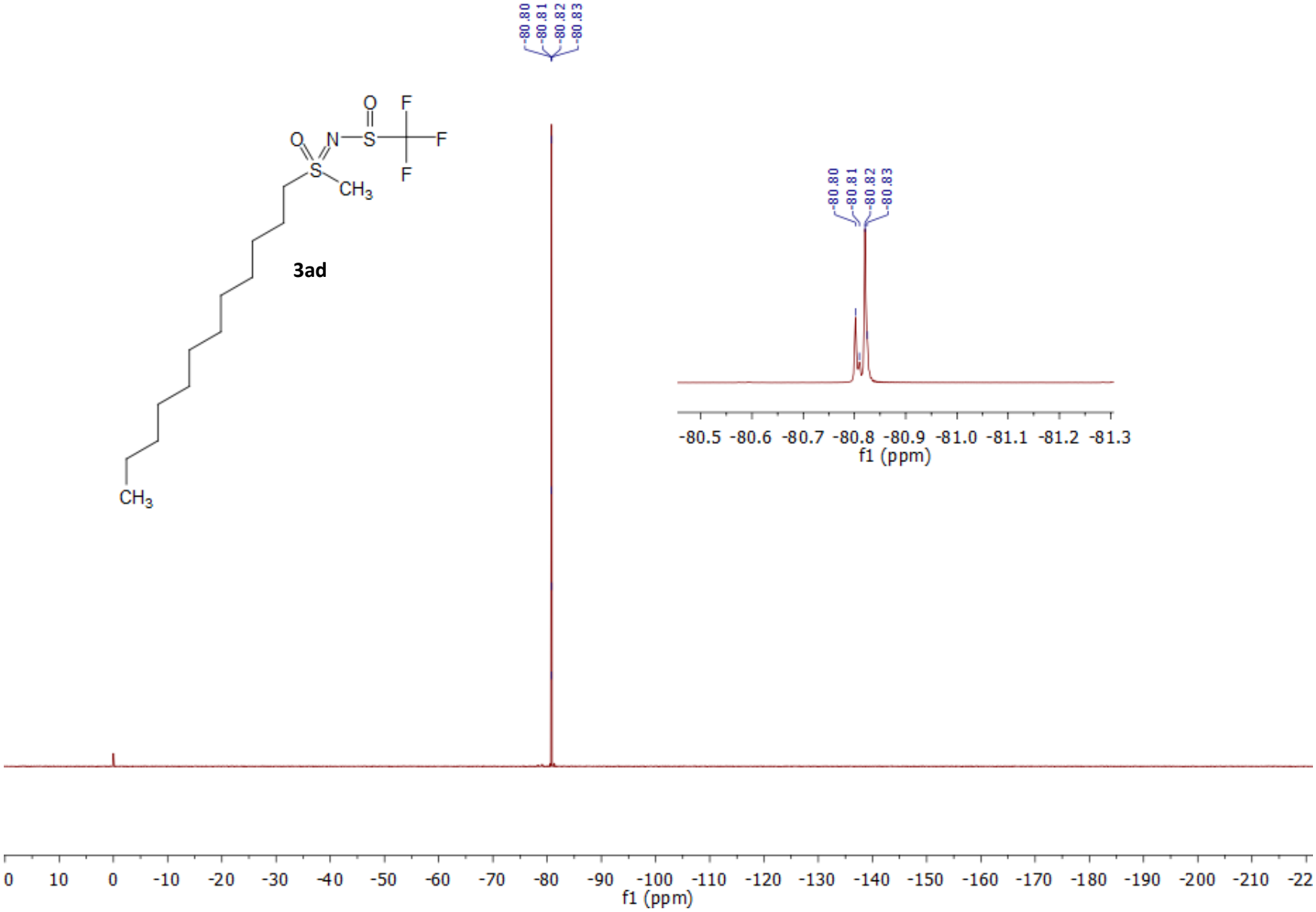
O
F
S
O
N
S
F
S
F
N
CH3

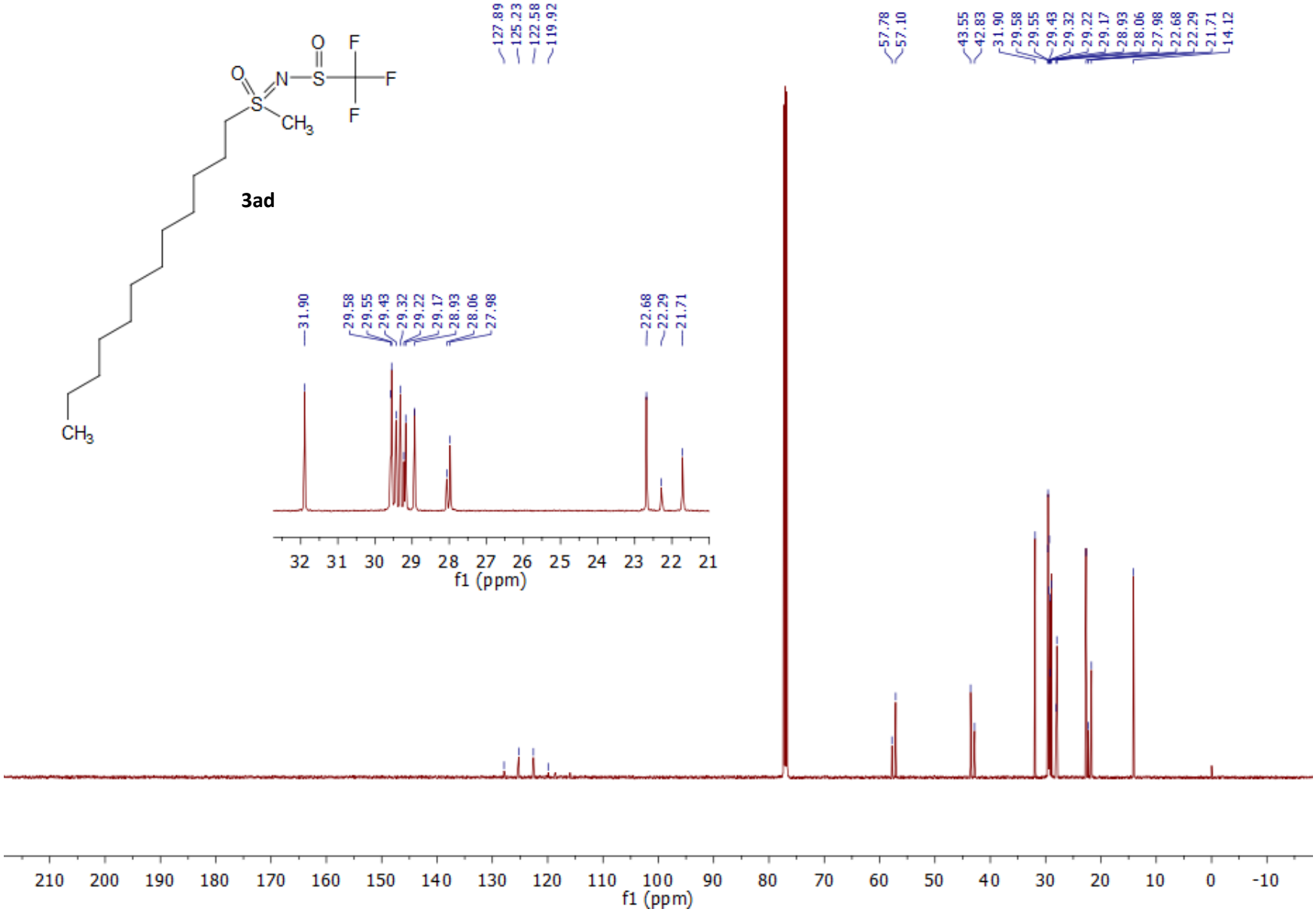
3ac

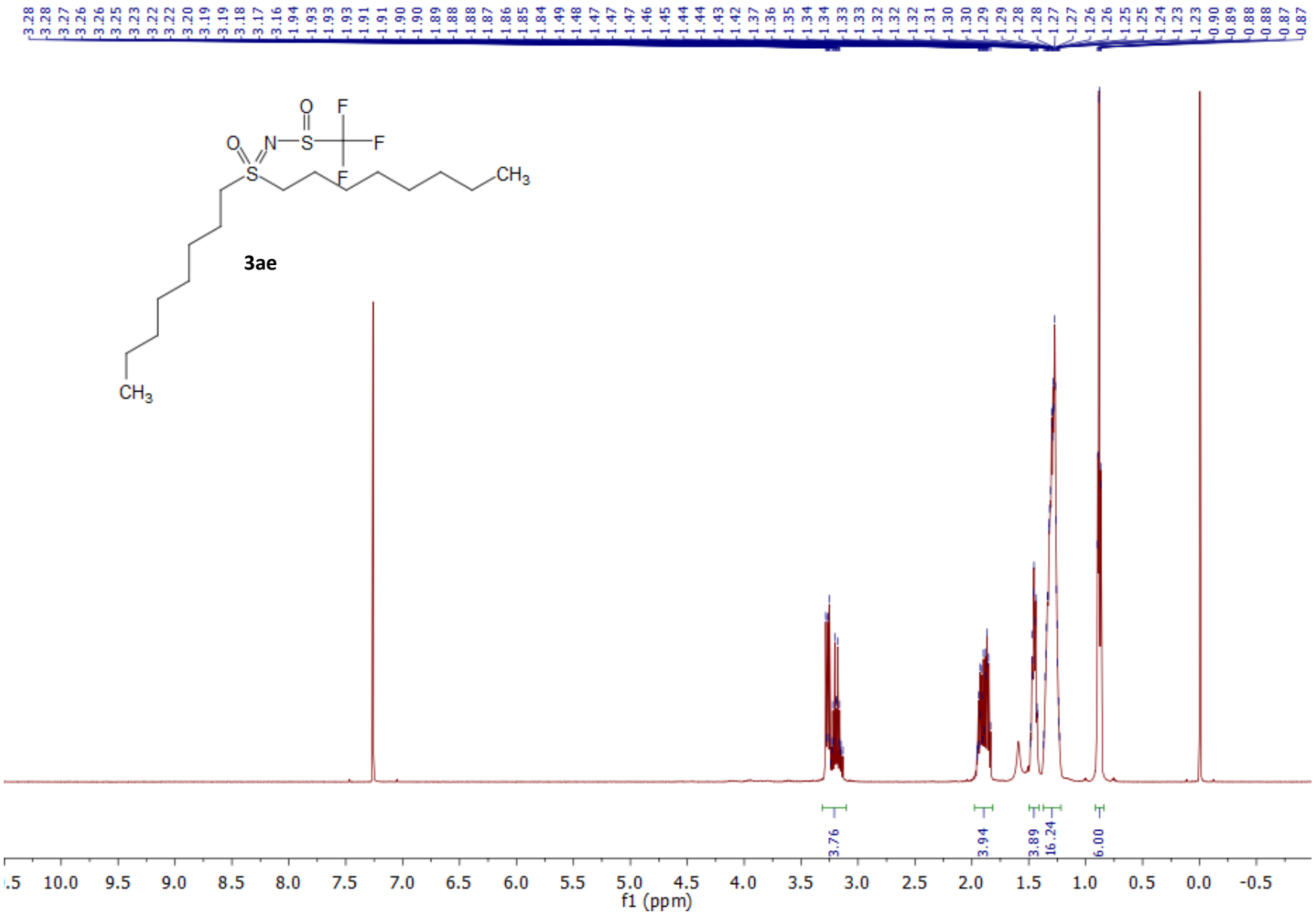

-80.28
-80.40
-80.28
-80.40
-80.20
-80.25
-80.30
-80.35
-80.40
-80.45
f1 (ppm)
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

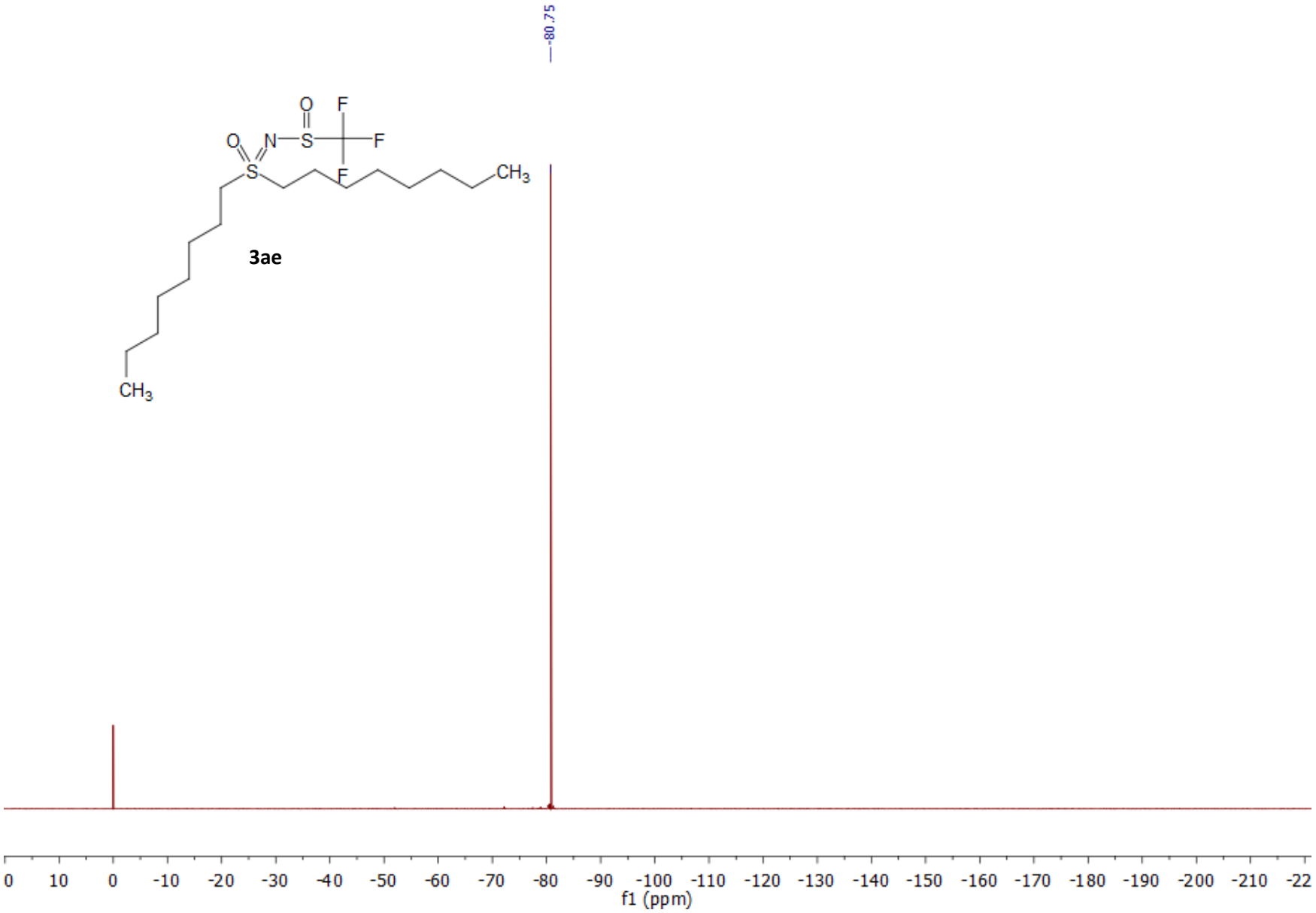

164.51
164.16
152.61
137.71
137.50
128.91
128.30
127.93
125.94
125.80
125.26
122.60
122.56
122.54
119.94
45.51
45.16
O
F
S
O
N
S
F
S
F
N
CH3
3ac
128.30
127.93
125.94
125.80
125.26
122.60
122.56
122.54
119.94
128 127 126 125 124 123 122 121 120 119
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

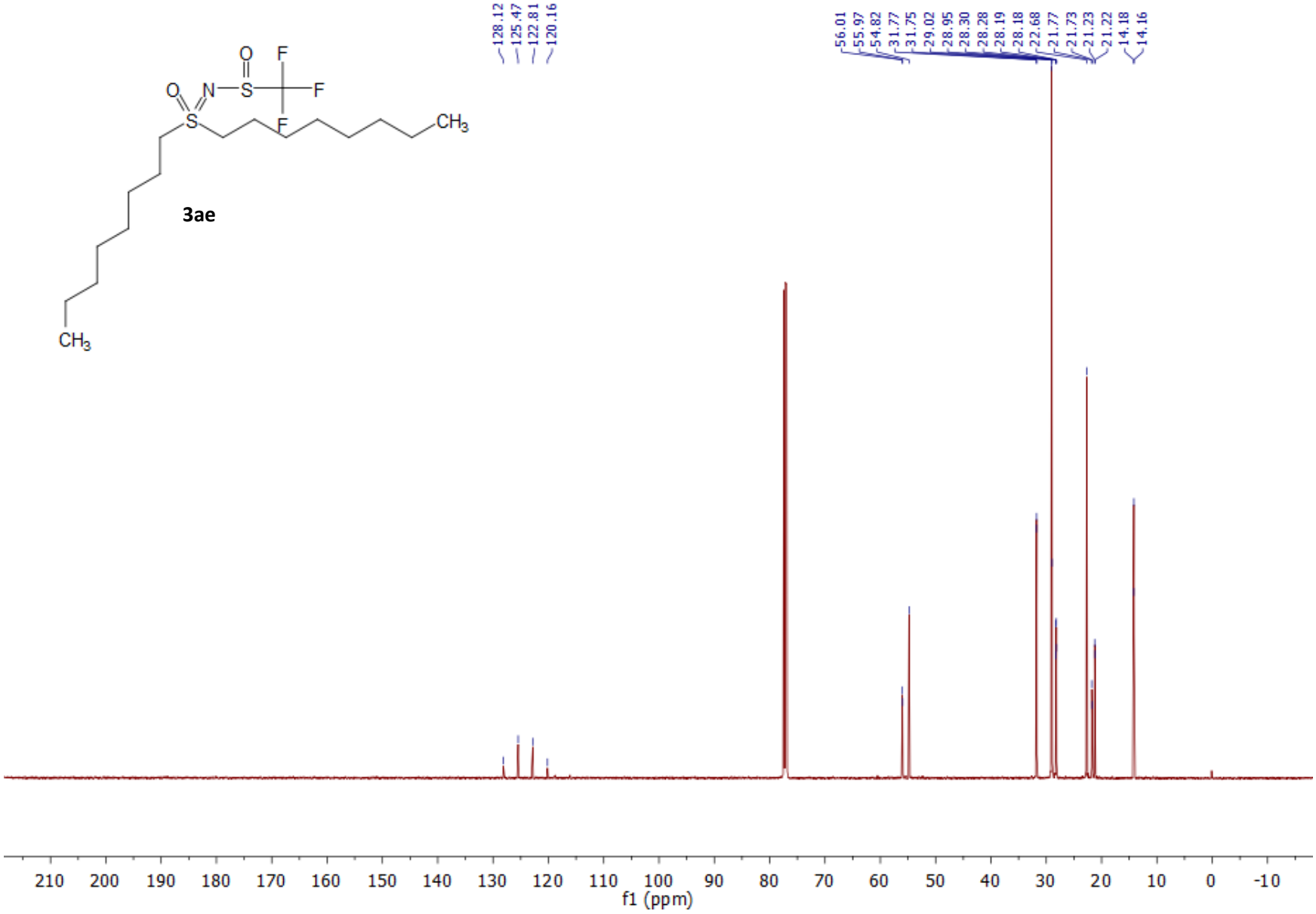

O
F
O
N
S
F
S
F
CH3
CH3
3ad
3.36
3.36
3.35
3.34
3.33
3.32
3.31
3.30
3.29
3.28
3.28
3.26
3.25
3.25
3.24
3.22
3.20
1.96
1.95
1.95
1.94
1.94
1.93
1.93
1.93
1.92
1.92
1.91
1.90
1.88
1.86
1.47
1.47
1.46
1.45
1.34
1.34
1.33
1.31
1.31
1.30
1.29
1.28
1.27
1.26
0.89
0.88
5.02
2.08
2.06
16.85
3.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

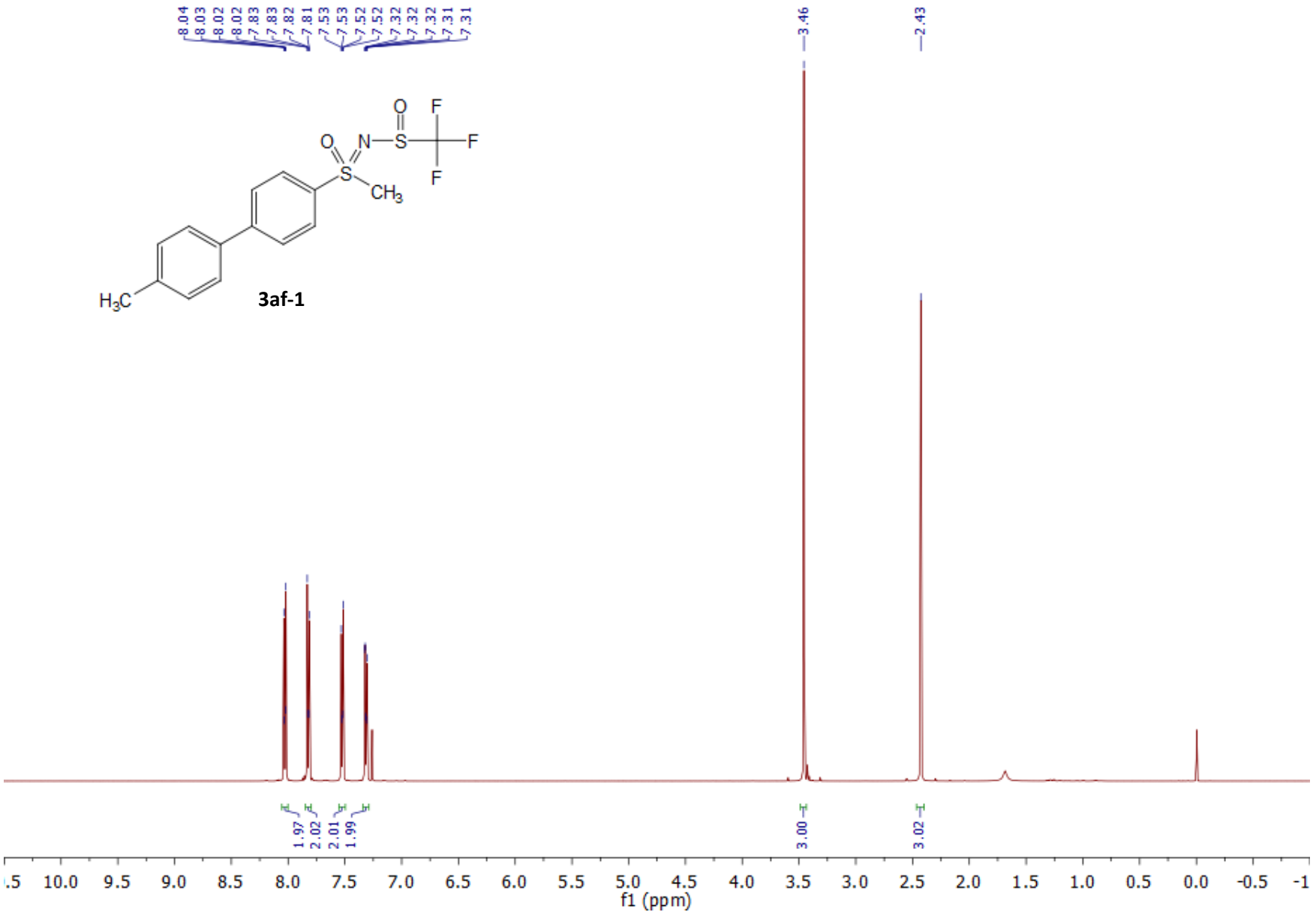

-80.80
-80.81
-80.82
-80.83
O
F
O
N
S
F
S
F
CH3
CH3
3ad
-80.80
-80.81
-80.82
-80.83
-80.5 -80.6 -80.7 -80.8 -80.9 -81.0 -81.1 -81.2 -81.3
f1 (ppm)
0 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)


127.89
125.23
122.58
119.92
57.78
57.10
43.55
42.83
31.90
29.58
29.55
29.43
29.32
29.22
29.17
28.93
28.06
27.98
22.68
22.29
21.71
14.12
O
F
O
N
S
F
S
CH3
F
CH3
3ad
31.90
29.58
29.55
29.43
29.32
29.22
29.17
28.93
28.06
27.98
22.68
22.29
21.71
32 31 30 29 28 27 26 25 24 23 22 21
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

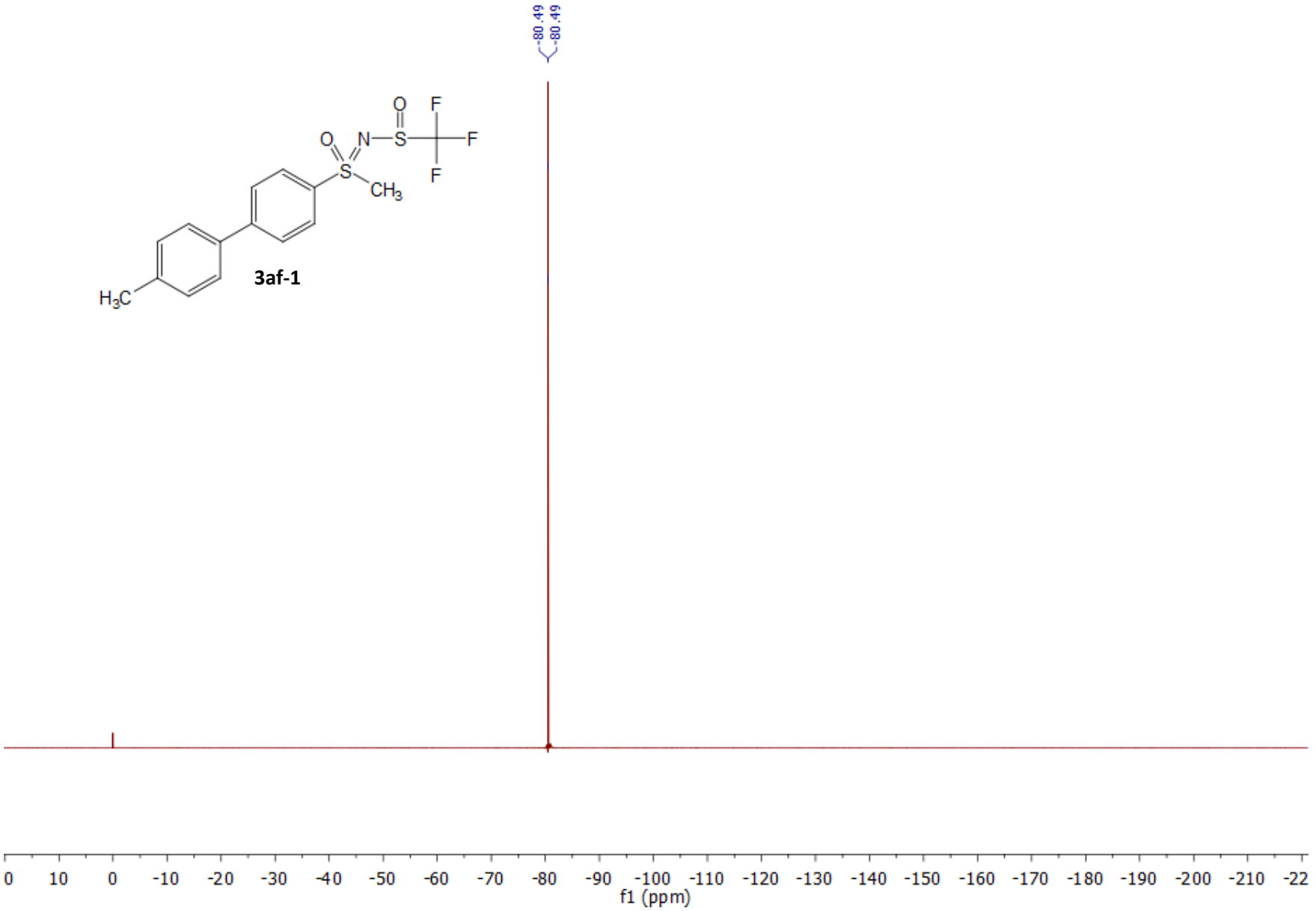

3.28 3.28 3.27 3.26 3.26 3.25 3.23 3.22 3.22 3.20 3.19 3.19 3.18 3.17 3.16 1.94 1.93 1.93 1.93 1.91 1.91 1.90 1.90 1.89 1.88 1.88 1.87 1.86 1.85 1.84 1.49 1.48 1.47 1.47 1.47 1.46 1.45 1.44 1.44 1.43 1.42 1.37 1.36 1.35 1.34 1.34 1.33 1.33 1.32 1.32 1.32 1.31 1.30 1.30 1.29 1.29 1.28 1.28 1.27 1.27 1.26 1.26 1.25 1.25 1.24 1.23 1.23 0.90 0.89 0.88 0.88 0.87 0.87
O F
O N S F
S F
CH3
CH3
3ae
3.76
3.94
3.89
16.24
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

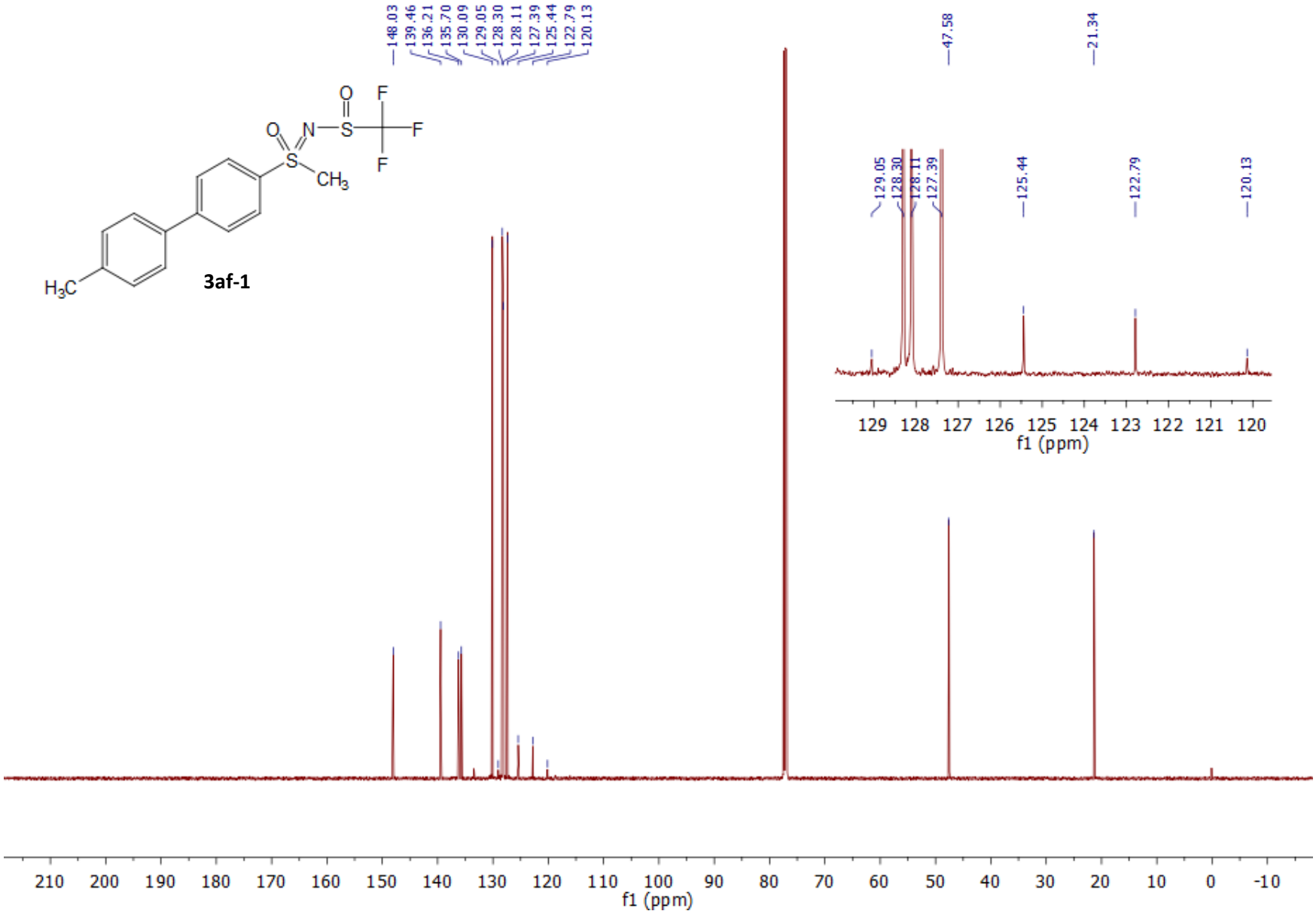

-80.75
O
F
O
N
S
F
S
F
CH3
CH3
3ae
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

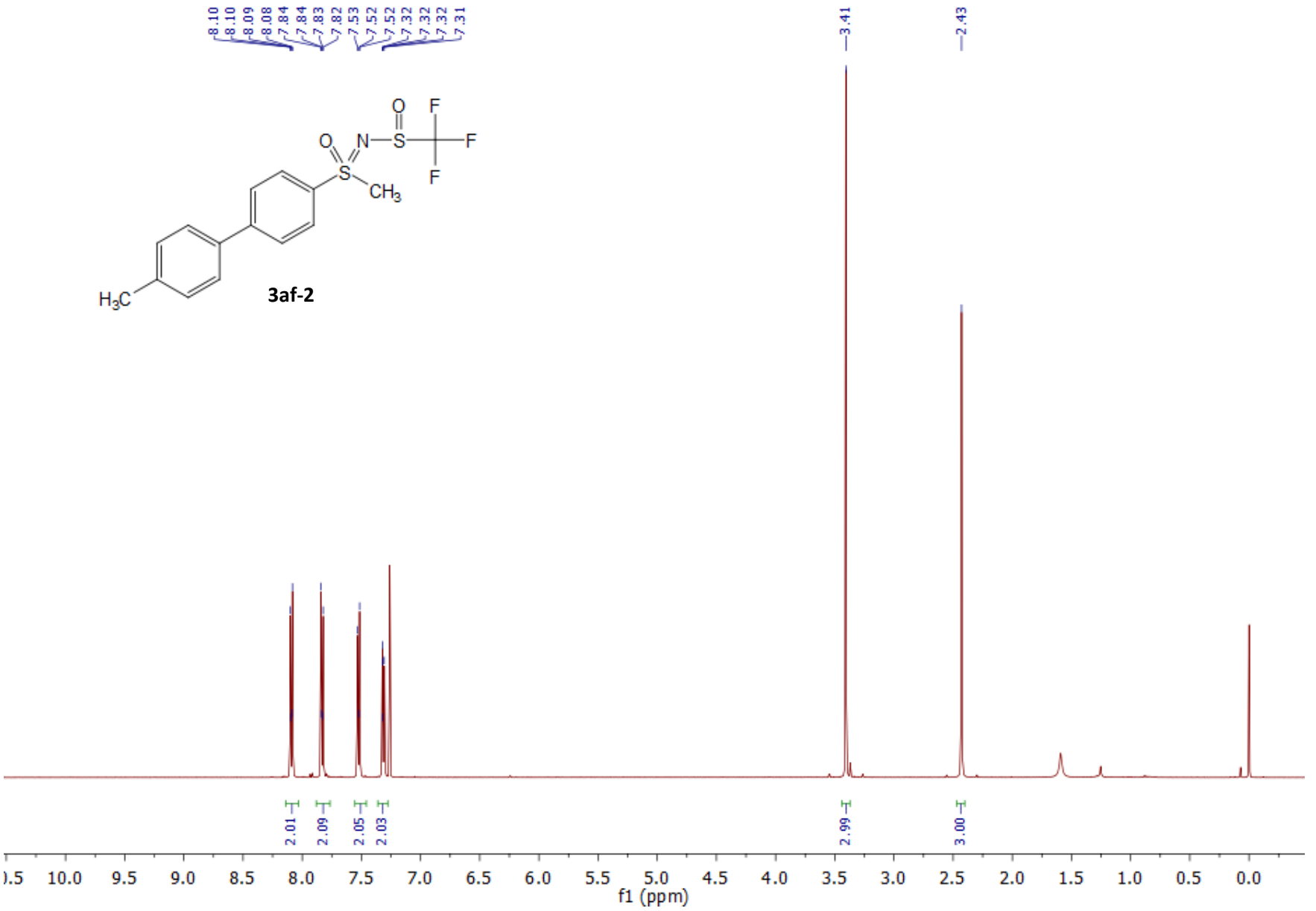

128.12
125.47
122.81
120.16
56.01
55.97
54.82
31.77
31.75
29.02
28.95
28.30
28.28
28.19
28.18
22.68
21.77
21.73
21.23
21.22
14.18
14.16
O
F
O
N
S
F
S
F
CH3
CH3
3ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.04
8.03
8.02
8.02
7.83
7.83
7.82
7.81
7.53
7.53
7.52
7.52
7.32
7.32
7.32
7.31
7.31
3.46
2.43
O
F
O
N
S
F
S
F
CH3
H3C
1.97
2.02
2.01
1.99
3.00
3.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

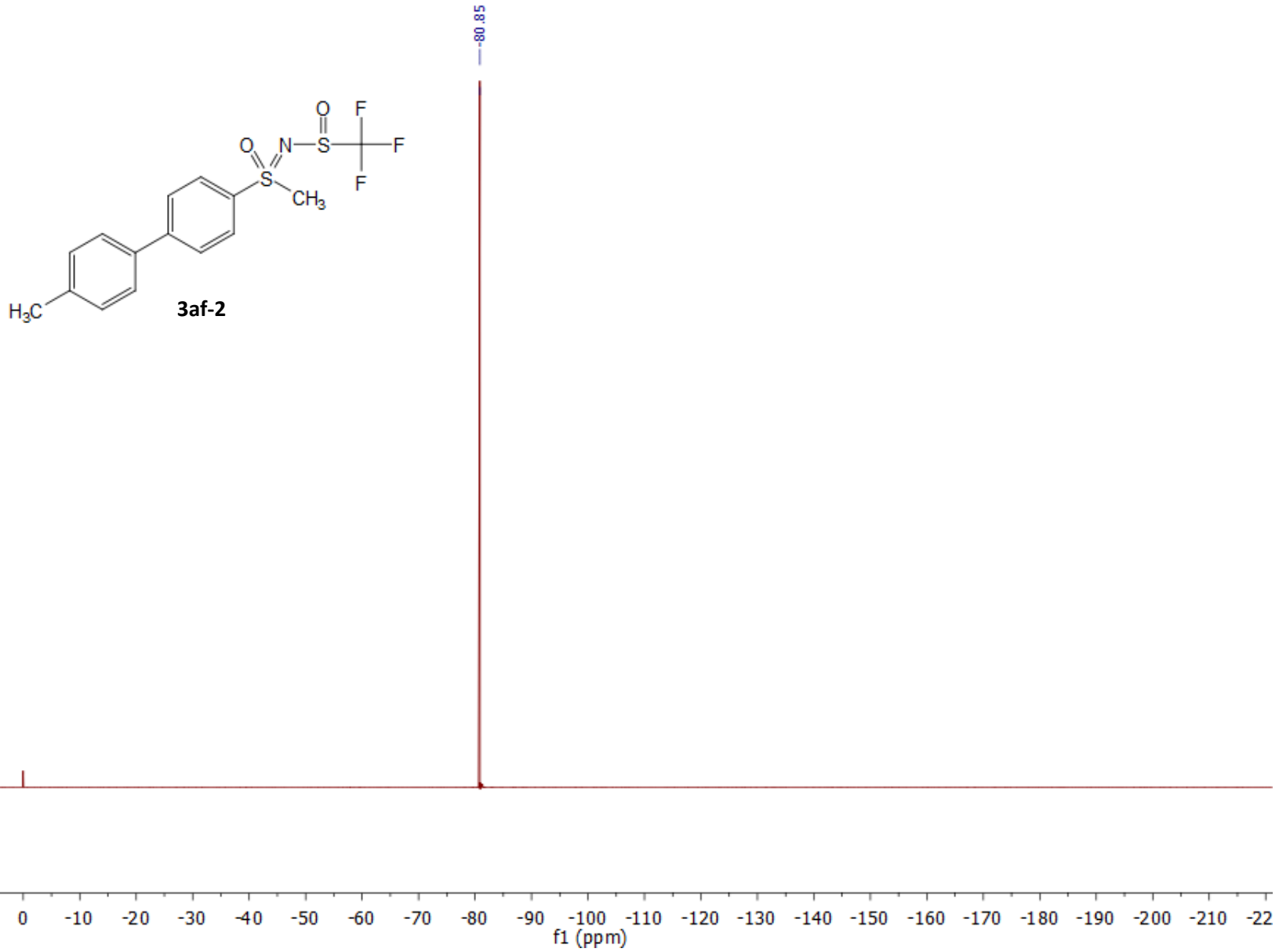
3af-1


-80.49
-80.49
O
F
O
N
S
F
S
F
CH3
H3C
3af-1
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

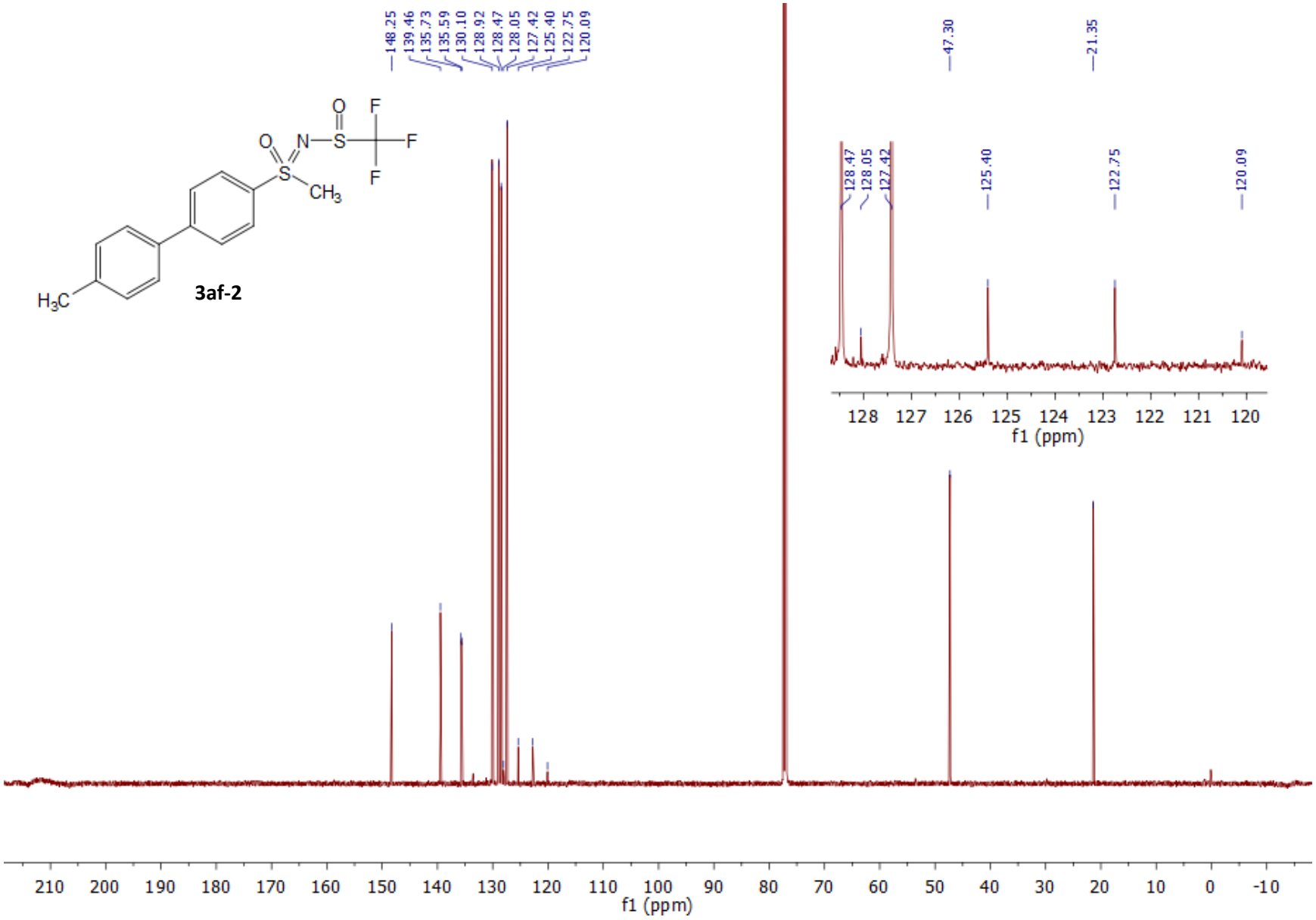

148.03
139.46
136.21
135.70
130.09
129.05
128.30
128.11
127.39
125.44
122.79
120.13
47.58
21.34
O
F
O
N
S
F
S
F
CH3
H3C
3af-1
129.05
128.30
128.11
127.39
125.44
122.79
120.13
129 128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

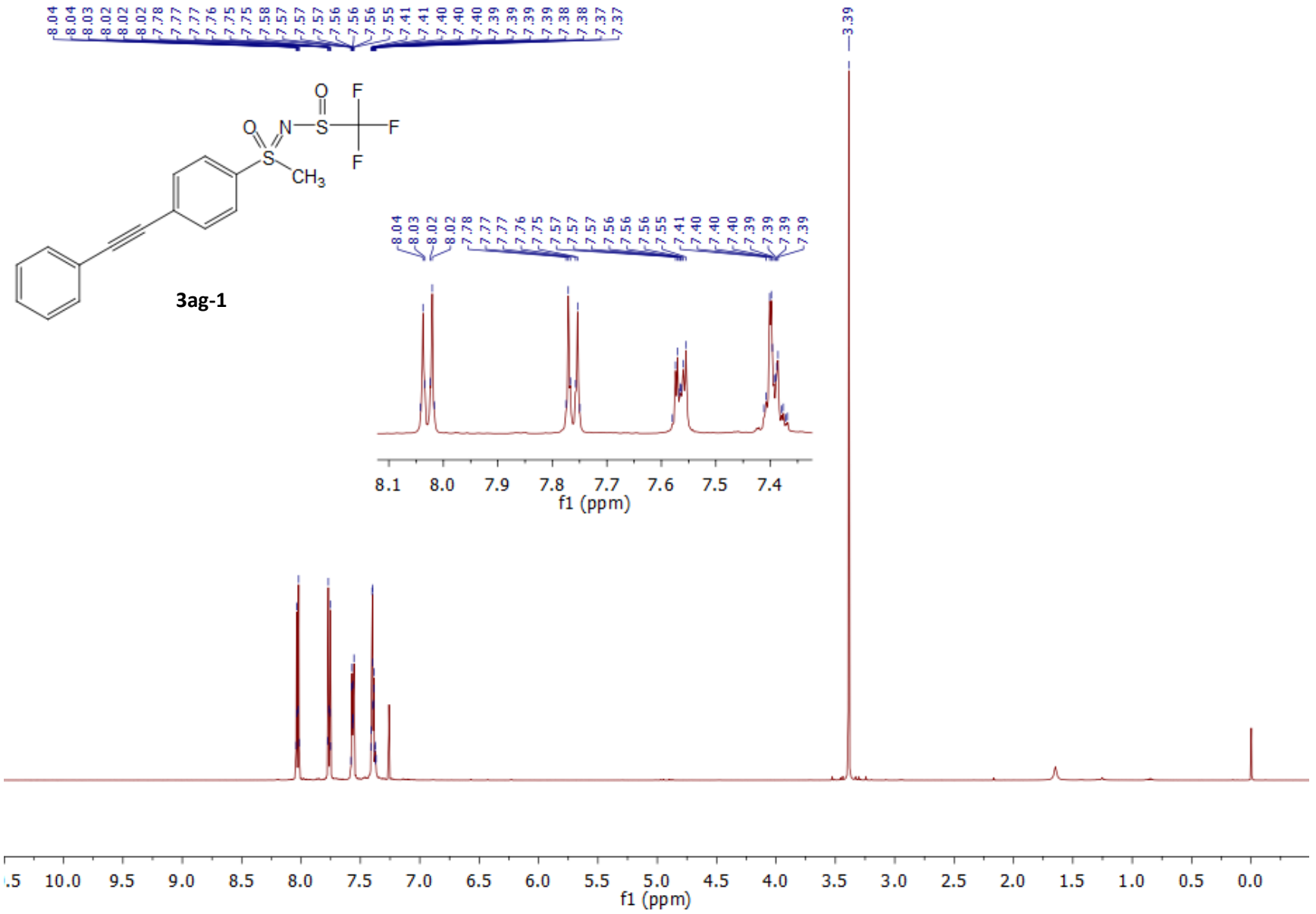

8.10
8.10
8.09
8.08
7.84
7.84
7.83
7.82
7.53
7.52
7.52
7.32
7.32
7.32
7.31
3.41
2.43
O
F
O
N
S
F
S
F
CH3
H3C
2.01
2.09
2.05
2.03
2.99
3.00
f1 (ppm)

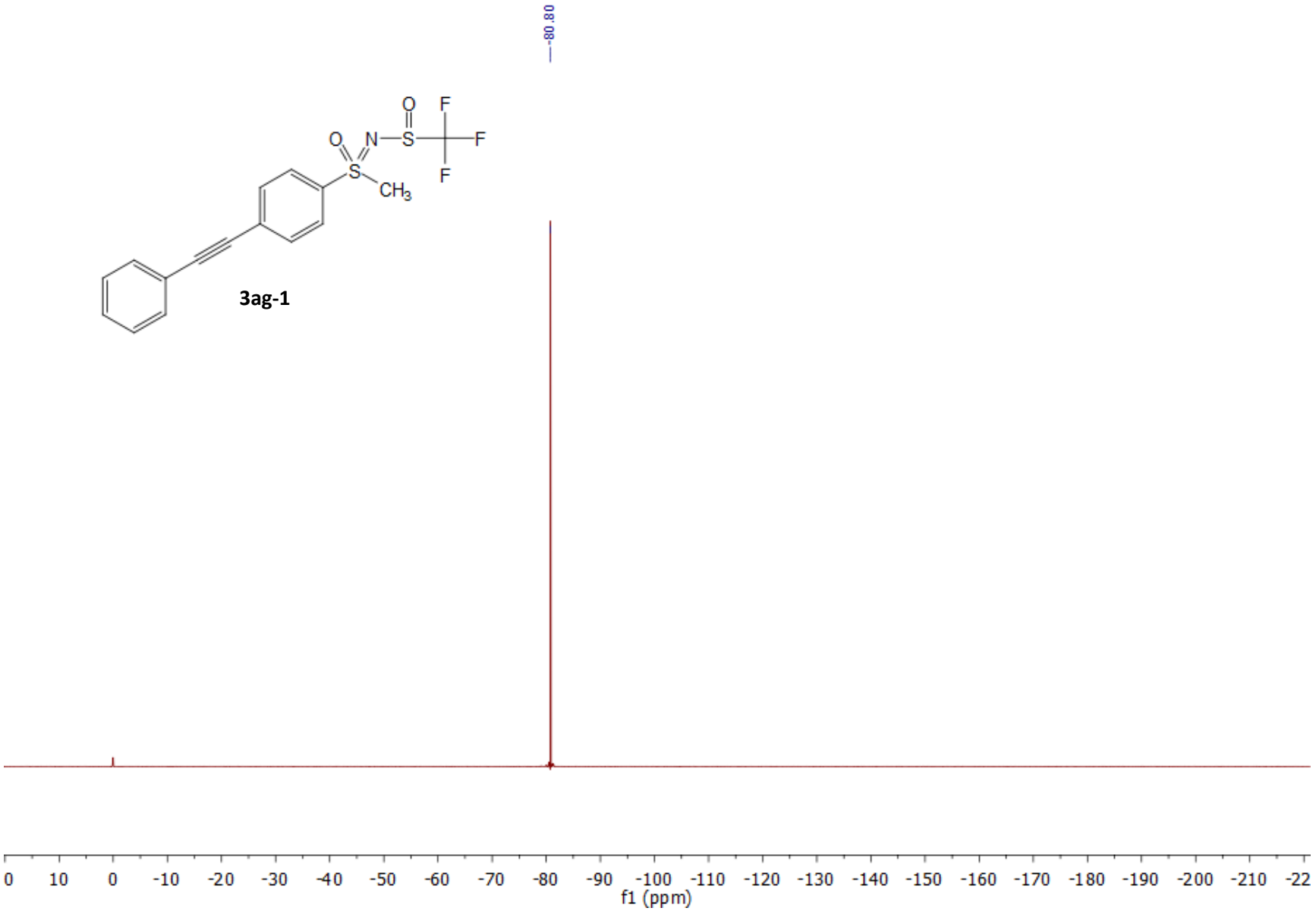
3af-2

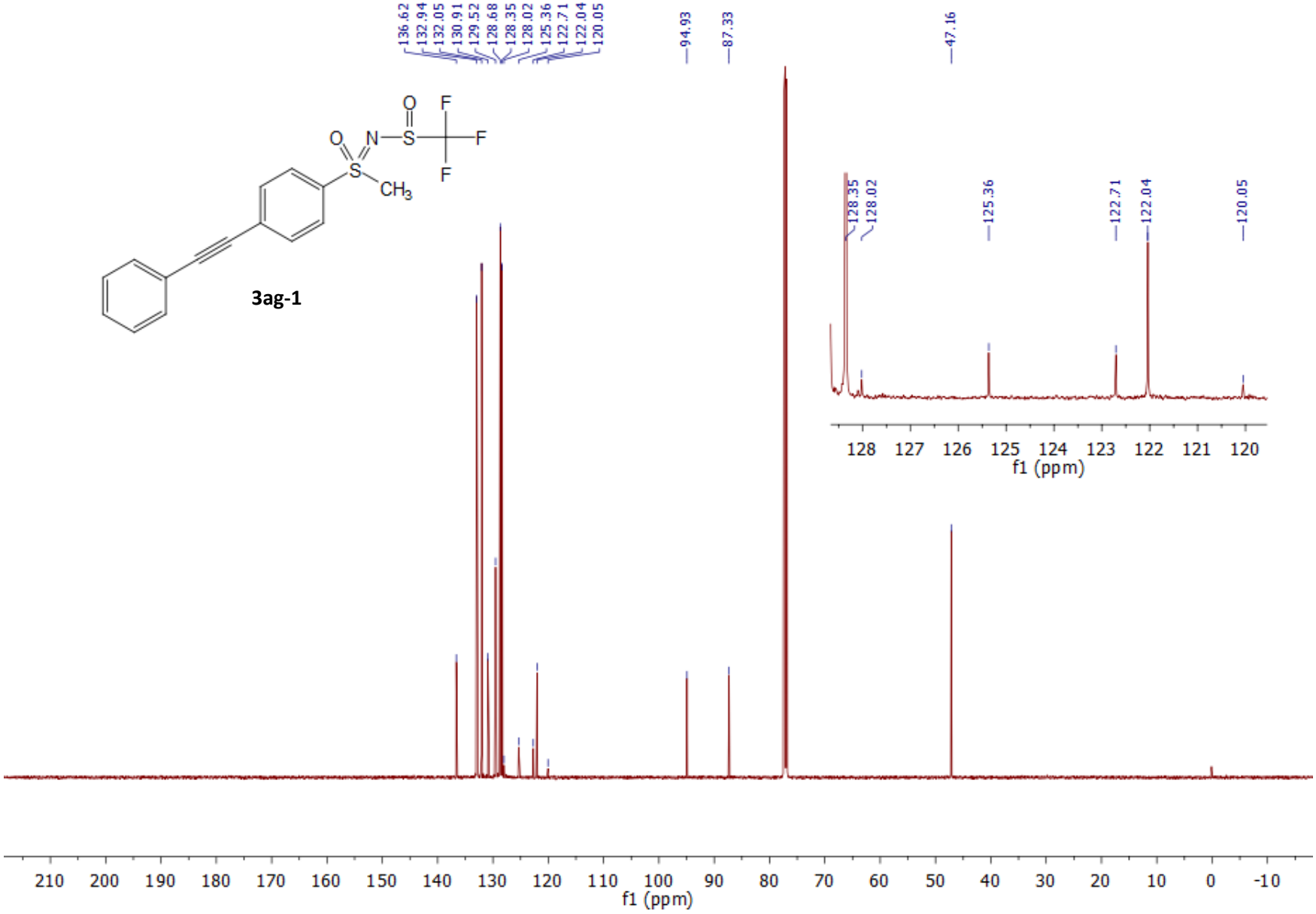

-80.85
O
F
O
N
S
F
S
F
CH3
H3C
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

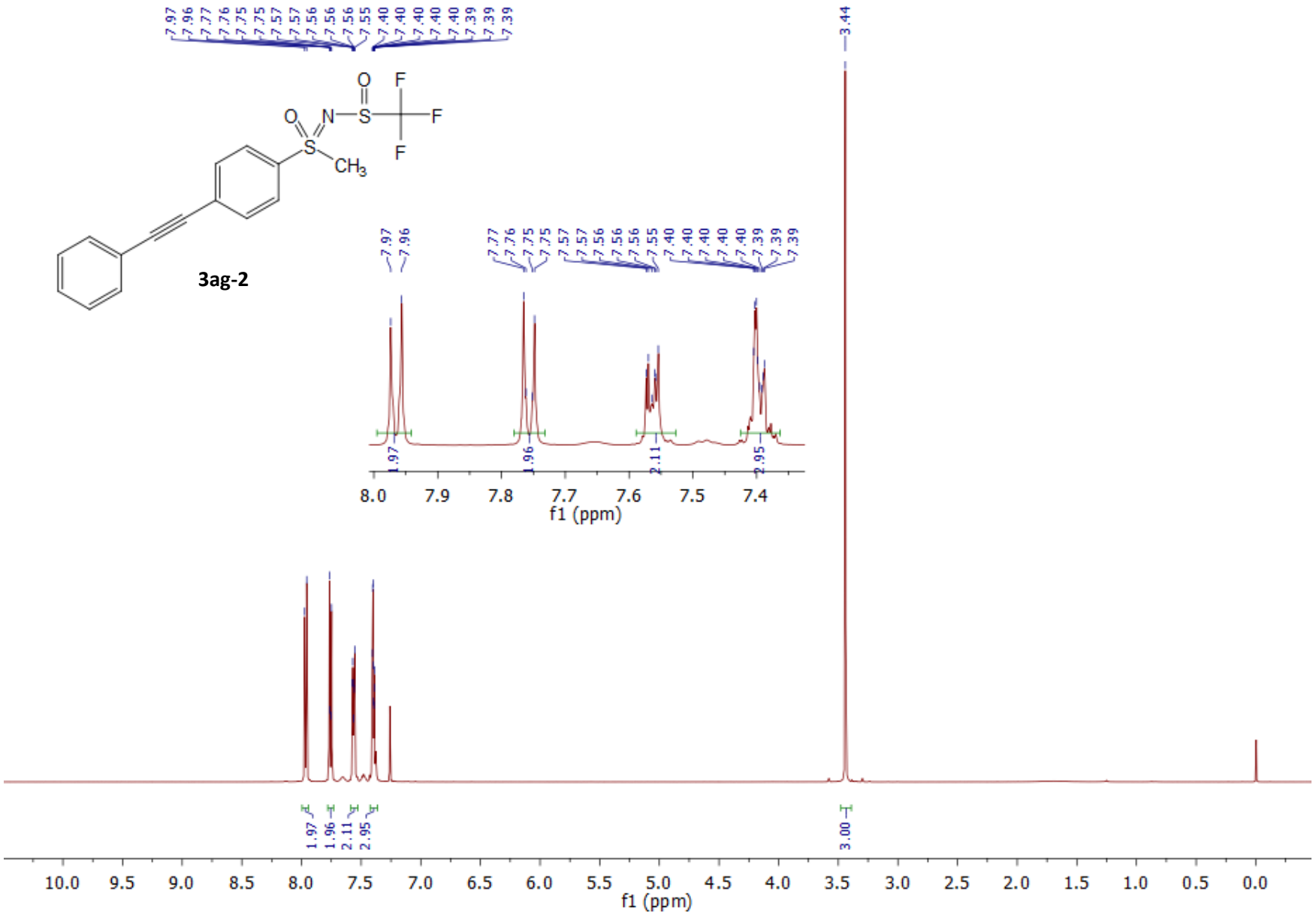
3af-2

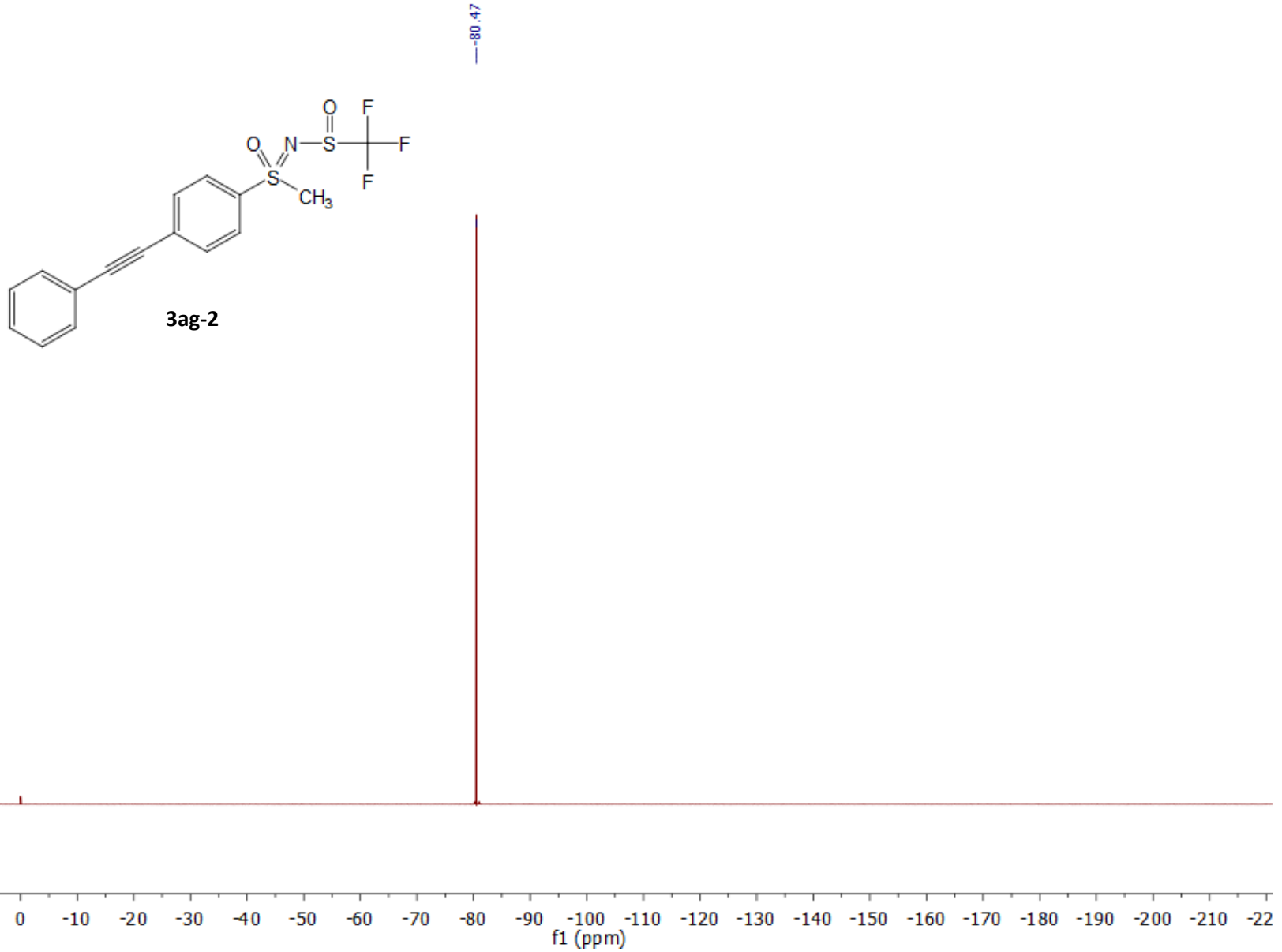

148.25
139.46
135.73
135.59
130.10
128.92
128.47
128.05
127.42
125.40
122.75
120.09
47.30
21.35
O
F
O
N
S
F
S
F
CH3
H3C
3af-2
128.47
128.05
127.42
125.40
122.75
120.09
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.04 8.04 8.03 8.02 8.02 8.02 7.78 7.77 7.77 7.76 7.75 7.75 7.58 7.57 7.57 7.57 7.56 7.56 7.56 7.55 7.41 7.41 7.40 7.40 7.40 7.39 7.39 7.39 7.39 7.38 7.37 7.37
3.39
O F
O N S F
S F
CH3
3ag-1
8.04 8.03 8.02 8.02 7.78 7.77 7.77 7.76 7.75 7.57 7.57 7.57 7.56 7.56 7.56 7.55 7.41 7.40 7.40 7.40 7.39 7.39 7.39 7.39
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)
.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

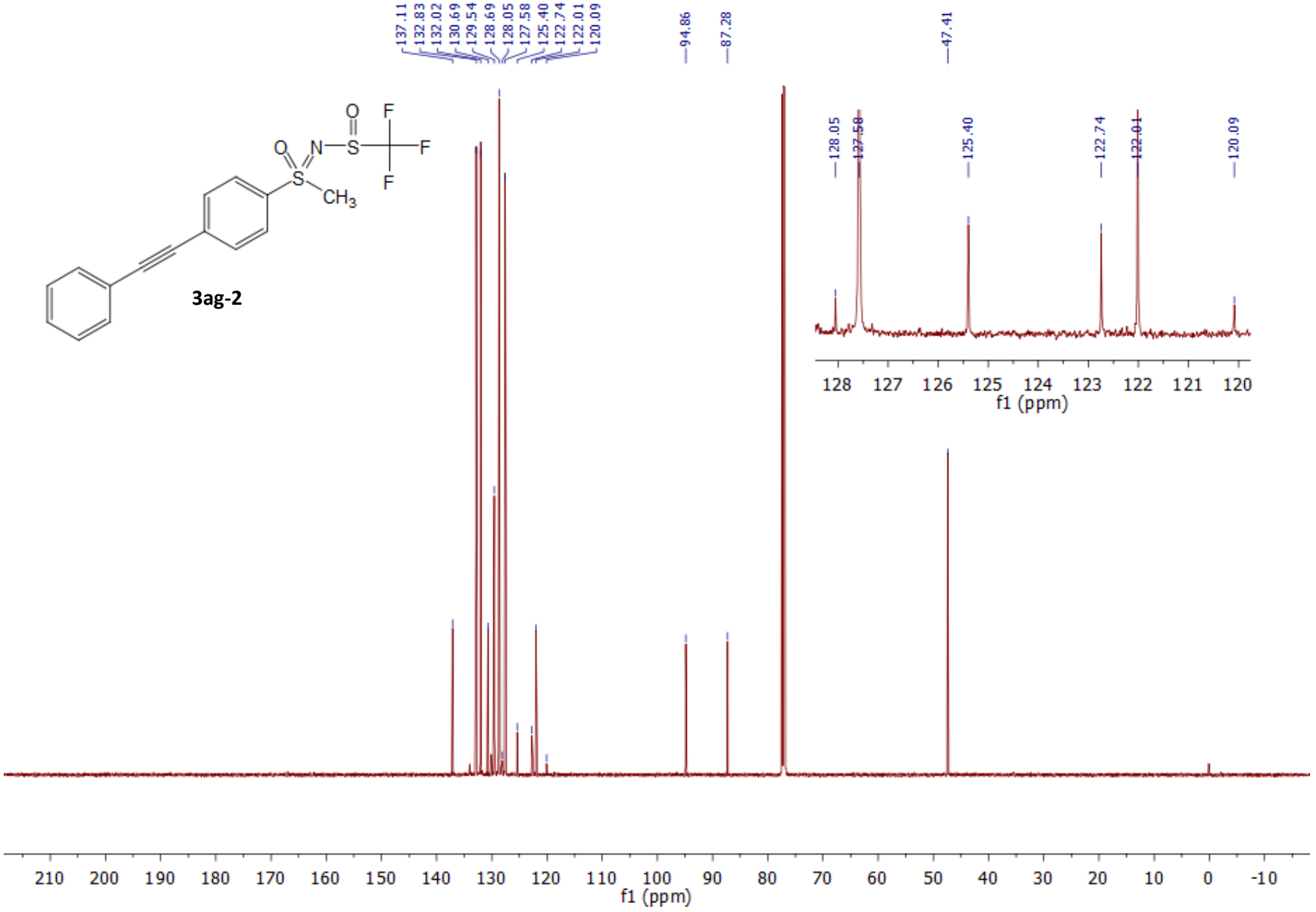

-80.80
O
F
O
N
S
F
S
F
CH3
3ag-1
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

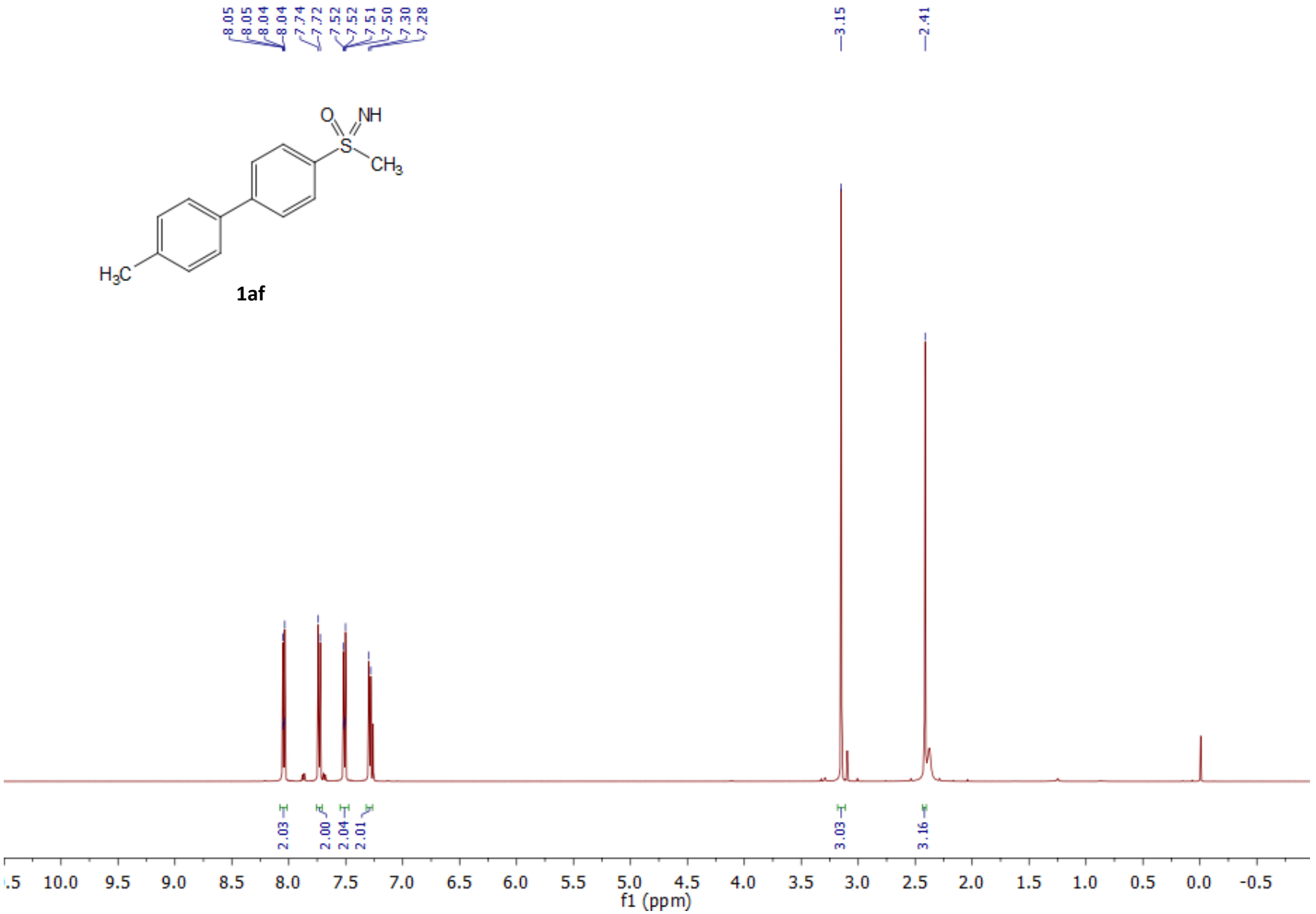

136.62
132.94
132.05
130.91
129.52
128.68
128.35
128.02
125.36
122.71
122.04
120.05
94.93
87.33
47.16
O
F
O
N
S
F
S
F
CH3
3ag-1
128.35
128.02
125.36
122.71
122.04
120.05
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.97
7.96
7.77
7.76
7.75
7.75
7.57
7.57
7.56
7.56
7.55
7.40
7.40
7.40
7.40
7.39
7.39
7.39
3.44
O
F
O
N
S
F
S
F
CH3
3ag-2
1.97
1.96
2.11
2.95
8.0
7.9
7.8
7.7
7.6
7.5
7.4
f1 (ppm)
1.97
1.96
2.11
2.95
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

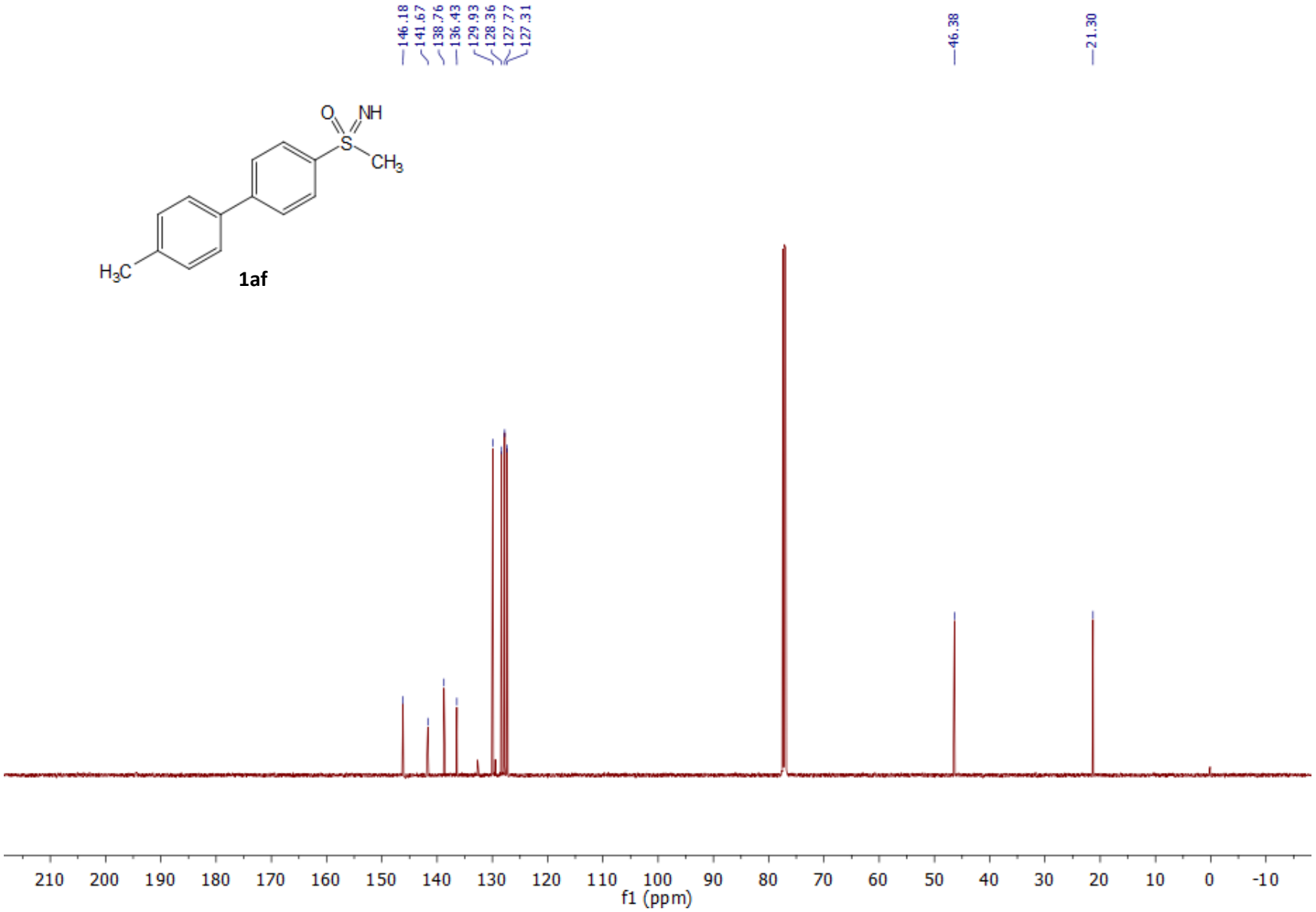

-80.47
O
F
O
N
S
F
S
F
CH3
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

3ag-2


137.11
132.83
132.02
130.69
129.54
128.69
128.05
127.58
125.40
122.74
122.01
120.09
94.86
87.28
47.41
O
F
O
N
S
F
S
F
CH3
3ag-2
128.05
127.58
125.40
122.74
122.01
120.09
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.05
8.05
8.04
8.04
7.74
7.72
7.52
7.52
7.51
7.50
7.30
7.28
3.15
2.41
O
NH
S
CH3
H3C
2.03
2.00
2.04
2.01
3.03
3.16
f1 (ppm)

1af


146.18
141.67
138.76
136.43
129.93
128.36
127.77
127.31
46.38
21.30
O
NH
S
CH3
H3C
1af
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)